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Disclaimer:

Thermomechanical Modeling of Hydride Materials for Tritium Storage Beds

This project aims to develop a fundamental modeling capability suitable for the simulation and assessment of various hydride materials and their associated storage vessels and deuterium/tritium delivery methods. If successful, this work will:

- ***Enhance*** a core competency of SRNL by adding a unique capability to the tritium processing R&D efforts currently performed for NNSA Defense Programs
- ***Optimize*** the design and operation of future hydrogen storage technologies in anticipation of increased demands and the call for a robust, reliable, resilient, and responsive stockpile
- ***Establish*** SRNL as a valuable analytic resource for DOE and DoD decision makers and the foreign technology assessment community, which has already shown significant interest in developing such models to assess the likelihood and feasibility of alternative foreign gas (deuterium/tritium) storage and delivery systems that might provide new technical pathways for the U.S. and to determine the performance of alternative foreign systems.

Awards and Recognition

N/A

Intellectual Property Review

This report has been reviewed by SRNL Legal Counsel for intellectual property considerations and is approved to be publicly published in its current form.

SRNL Legal Signature

Signature **Date**

Thermomechanical Modeling of Hydride Materials for Tritium Storage Beds

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Thrust Area: National Security

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U.S. analysts currently have a very limited understanding of hydride materials potentially used by other nuclear weapon states for the storage and delivery of tritium and deuterium. The ability to model such hydride materials and their associated storage beds would provide a unique fundamental capability to SRNL in support of multiple programs in National Security. This capability will provide a competitive advantage relative to other DOE Laboratories and a collateral benefit for the SRNL Tritium processing mission. The modeling capability is of interest to many sponsors that SRNL is currently engaged with. This capability will leverage and expand upon a key core competency of the National Security Directorate.

FY2018 Objectives

- Conduct extensive foreign database open literature search for hydride materials used for deuterium/tritium storage, particularly those engaged by Russian scientists, whom we assume would have the most to offer in terms of technical alternatives
- Leverage network analysis techniques to identify important connections within Russia's metal hydride research and development community – individual contributors, associated institutions, and funding agencies
- Identify candidate hydride material(s) of interest and begin collecting characterization data as the basis for a phenomenological model of its storage and delivery performance

Introduction

U.S. analysts, technologists, and programmatic decision makers currently have a very limited understanding of the hydride materials used in foreign systems for the storage and delivery of deuterium and tritium. The fundamental properties of hydride storage materials affect storage vessel/bed and weapon performance, associated maintenance intervals (decay and He-3 retention), required production capacity, and required tritium delivery pressures/rates. At elevated temperatures, hydrogen reacts with many transition metals to form hydrides. The lanthanides, actinides, members of the titanium and vanadium groups, scandium, and yttrium as well as their associated alloys are the most reactive toward hydrogen absorption.[1] The absorption/desorption behavior of metal hydrides is most commonly measured by isothermal pressure-composition response curves (isotherms), in which the material undergoes a phase transition (α→β or vice versa) as hydrogen is either absorbed or desorbed. The transition is demonstrated in the isotherm by the length and slope of the plateau region, which are indicative of the capacity and homogeneity of the hydride, respectively. A schematic of a typical two-phase isotherm is given in Figure 1.[2]

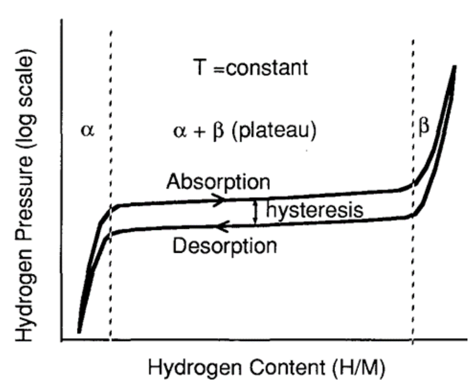


Figure 1. General absorption/desorption isotherm

The thermodynamic properties of metal hydride formation from gaseous hydrogen can determined by the collection of isotherms at various temperatures. The series of isotherms can be used to calculate the enthalpy (ΔH) and entropy (ΔS) for the absorption and desorption of the hydrogen using the equilibrium pressure and the van't Hoff equation:

$$ln\frac{P_{eq}}{P_{eq}^{0}} = \frac{\Delta H}{R} \times \frac{1}{T} - \frac{\Delta S}{R}$$

A schematic of hydrogen absorption and a general van't Hoff plot is shown in Figure 3, where the enthalpy (ΔH) and entropy (ΔS) of reaction are given by the slope and y-intercept of the line, respectively.

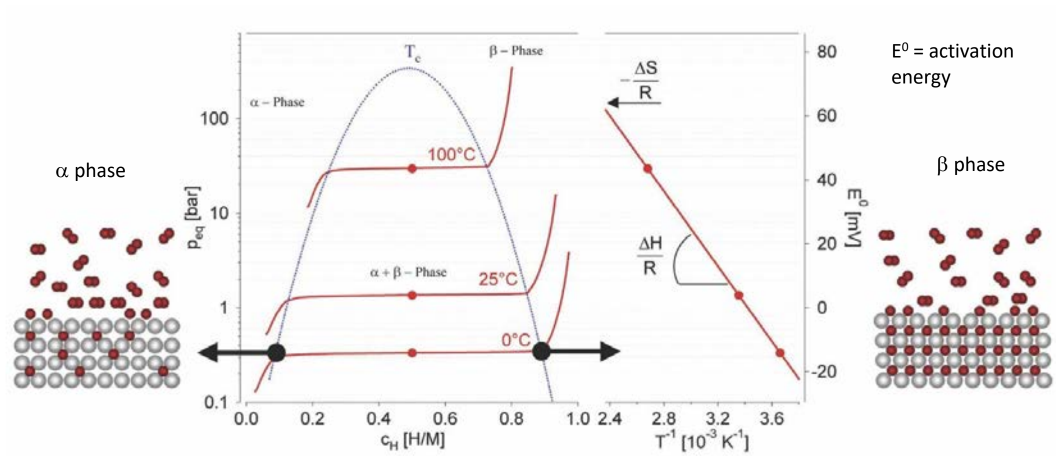


Figure 2. *Schematic of hydrogen absorption and van't Hoff plot.*

Alternate storage materials potentially used in other countries may perform better (in terms of absorption/desorption rates, storage capacity, He-3 retention, etc.) – or differently, in ways we should understand – than the current hydride materials used by the United States. Understanding hydride storage materials and their application to tritium storage and delivery is a core competency of SRNL and an area of recognized expertise for SRNL within the U.S. foreign technology analytical community (albeit, in competition with the nuclear design laboratories). Expanding our understanding of hydride materials used by other nuclear-weapon states will enhance an SRNL core competency and establish a strategic capability to assess new technology opportunities as well as the capabilities of other nations.

This project aims to develop a fundamental modeling capability suitable for the simulation and assessment of various hydride materials and their associated storage vessels and deuterium/tritium delivery methods. If successful, this work will:

- ***Enhance*** a core competency of SRNL by adding a unique capability to the tritium processing R&D efforts currently performed for NNSA Defense Programs
- ***Optimize*** the design and operation of future hydrogen storage technologies in anticipation of increased demands and the call for a robust, reliable, resilient, and responsive stockpile
- ***Establish*** SRNL as a valuable analytic resource for DOE and DoD decision makers and the foreign technology assessment community, which has already shown significant interest in developing such models to assess the likelihood and feasibility of alternative foreign gas (deuterium/tritium) storage and delivery systems that might provide new technical pathways for the U.S. and to determine the performance of alternative foreign systems

Approach

The primary objective of this work is to focus on the research of Russian scientists to identify alternative metal hydride storage materials of interest and to develop a phenomenological model to simulate the performance of these hydride materials and their associated storage system. The first step toward this goal was an extensive literature search of hydride storage materials involved in tritium research and development in Russia. After thorough review of historical data, conference proceedings, and standard open literature sources, SRNL compiled a comprehensive list of search terms, including field-specific technical terms as well as individual contributors and institutions of interest. The search criteria were then applied to foreign databases by an expert network data analyst at the James Martin Center for Nonproliferation Studies with access to and expertise in various foreign databases. Next, a multi-modal network analysis of the resulting dataset was performed to provide insight into the overall structure of Russia's tritium storage research network. In addition to revealing potential hydride materials of interest for further study, this approach also provided valuable information on the institutions, funding agencies, and individuals engaging such materials in applied tritium research in Russia.

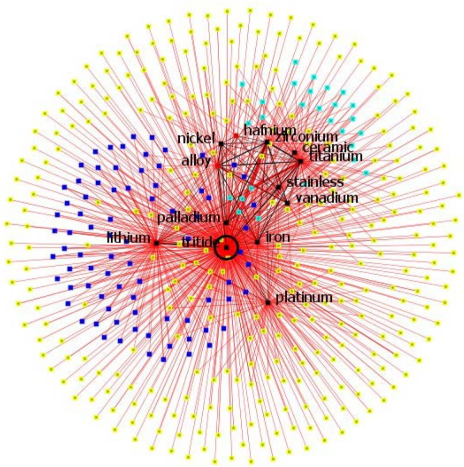
The hydride materials of interest will then be synthesized or obtained for further characterization. Depending on the rarity of the material(s), much of their hydrogen storage and delivery properties may already be known in the literature. If not, pressure-composition-temperature (PCT) response curves will be measured using protium and deuterium on existing test manifolds at SRNL, designed specifically for generating such data. The absorption/desorption performance, thermodynamic properties, and He-3 retention capability of the materials can then be used to predict the vessel parameters (e.g., wall thickness, heat load, pressure rating, tritium desorption/generation rate) required for operation in an engineered storage system. Finally, the developed models simulating the performance of the hydride materials and their associated storage vessels can be integrated to assess the capabilities of possible foreign systems and their applications. This approach leverages SRNL expertise and capabilities in metal hydride chemistry, tritium processing and storage, and national security studies and various activities within the intelligence community.

Results and Discussion

A thorough review of historical data, conference proceedings, open literature, and institutional knowledge was first performed to generate search criteria aimed at identifying potential alternatives to metal hydrides used at SRS. Field-specific terms (in both English and Russian) along with a list of individual researchers and institutions known for their work in this area were used as the basis for the initial foreign database bibliographic search. The broad scope of the initial search resulted in a dataset too large and noisy to draw any conclusions from. Thus, the search was narrowed down to focus on metals and/or materials in connection with either "tritide" or "deuteride" (and their Russian translations). This final iteration of the literature search resulted in a manageable dataset for further analysis. While the major findings are highlighted in the following paragraphs, the details of the literature search and subsequent multi-modal network analyses can be found in Appendix A - Hydrogen Solid-State Storage R&D in Russia.

Multi-modal network graphing techniques were then used to visualize the overall structure of the metal hydride research and development network in Russia, and highlight important connections between individual contributors, institutions, and funding agencies engaging materials of interest. Since there were no major surprises as far as the institutions, agencies, or individuals engaged in this field of research, the focus shifted toward the connection to specific metals and metal alloys being used. The large dataset revealed several materials of interest, including various vanadium (V) and titanium (Ti) alloys, for further investigation – some of which have been previously studied or are easily obtainable at SRNL. Of interest is Ti-Al6-V4, which is a powder alloy currently being used in SRNL's metal additive manufacturing (AM)

(a)



(b)

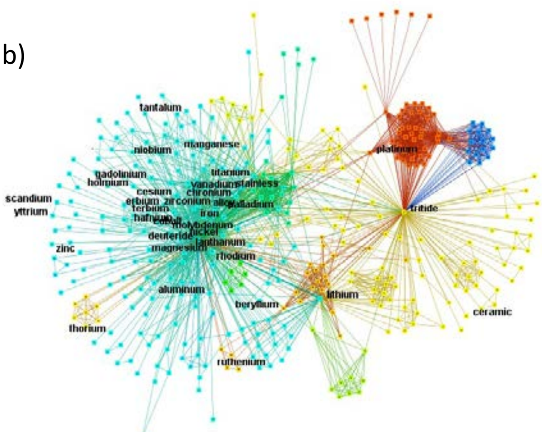


Figure 3. (a) "Tritide" 1st degree network with CONCOR grouping, which attempts to identify groups that are structurally similar. (b) Aggregate network with strong ties and Newman clustering, which attempts to identify local communities within a network.

machine. Pure titanium has been extensively studied at SRNL for its applications in long-term tritium storage,[3] but little is known about the tritium storage performance of its alloys. Work has begun to obtain materials of interest and collect hydrogen absorption/desorption data (if not known in the literature) to use as the basis for a phenomenological model of hydrogen storage and delivery performance.

In addition to revealing potential materials of interest, the network graphing also provided valuable insight into the "tritide" and "deuteride" research efforts in Russia. There was limited technical overlap observed between materials associated with "tritide" and "deuteride" research, which leads to other questions regarding the potential transition from fundamental to applied tritium research. The "tritide" network (shown in Figure 3a) was also found to include fewer material connections and be far less complex than the "deuteride" network. Moreover, a clear divide is observed in the "tritide" network between those working with platinum and those focusing on other materials, which is clearly delineated in the aggregate network shown in Figure 3b.

Other noteworthy items from this work include specific designs/materials for hydrogen storage vessels. For example, the details of a Russian "tritium generator" device (likely using uranium as the tritium storage medium) were found, which may provide insight into other tritium storage and delivery materials, container designs, and associated applications. Additionally, several papers on non-porous ceramic materials for induction heating were discovered, which may help support recent and ongoing R&D efforts at SRNL regarding the potential benefits and feasibility of induction heating of metal hydride vessels.

FY2018 Accomplishments

- Completed extensive open-source foreign database search using SRNL-generated criteria, focused on materials found in connection with "tritide" and "deuteride" search terms.
- Utilized multi-modal network analysis technique to gain valuable insight into the scientific network involved in metal hydride research and development in Russia.
- Determined that the "tritide" network is far less complex than the "deuteride" network, with a clear divide observed between those working with platinum and those focusing on other materials.
- Identified several materials of interest, including various vanadium and titanium alloys, as well as novel hydride storage and delivery concepts for further investigation and baseline modeling efforts.

Future Directions

Material Characterization

- Obtain/fabricate/procure materials of interest (some already available at SRNL or commercially available) and collect known absorption/desorption data or measure PCT isotherms using protium and deuterium on existing hydride manifolds at SRNL.
- Develop/re-establish SRNL in-house capability to produce metal alloy and intermetallic hydride-forming material in research quantities.

Integrated Modeling

- Using the thermodynamic data, develop models to simulate the performance of hydride materials and their associated storage beds to predict vessel parameters, heat loads, and gas flow rates required for operation in an engineered storage system.
- Integrate storage component models (material performance and associated storage container) and run simulations to assess capabilities of possible foreign systems.

Data/Network Analysis

- Additional mining of bibliographic data is necessary to further parse out fields, researchers, papers, materials, groups, etc. of interest.
- Create a timeline of key term "hits" to determine surges and/or gaps in technical competencies or focus areas. This will effectively map the history of metal hydride research (associated with tritium storage and delivery) in Russia over last 70 years to investigate alignment with significant world events and predict current/future trends.
- Develop SRNL in-house capability for bibliographic network analysis to allow real-time interactive graphical analysis of networks.

References

1. Züttel, "Materials for Hydrogen Storage," Materials Today, Vol. 6, pp. 24-33, 2003
2. L. K. Heung, "RTF Hydride Bed Technical Operating Guide", WSRC-TR-93-140, 1993
3. L. K. Heung, "Titanium for Long-Term Tritium Storage", WSRC-TR-94-0596, 1994

Acronyms/Abbreviations

Al	Aluminum
AM	Additive manufacturing
DOE	Department of Energy
ΔH	Enthalpy
H/M	Hydrogen-to-metal ratio
He-3	Helium-3
NNSA	National Nuclear Security Administration
PCT	Pressure-composition-temperature
P_{eq}	Pressure at equilibrium
R	Ideal gas constant
ΔS	Entropy
Ti	Titanium
V	Vanadium

Appendix A

Hydrogen Solid-State Storage R&D in Russia

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This study examines the scientific networks engaged with metal hydrides and solid-state hydrogen storage techniques in Russia. This study leverages network analysis techniques to map the research and organizational entities through an investigation of the pertinent scientific literature. In doing this, the research probes a large dataset to identify entities and organizations pursuing research in deuteride and tritide research; the type of materials engaged; the connections between these researchers, research groups, and funding organizations; and the overall structure of the solid-state hydrogen storage research network. The goal of this line of investigation is to attempt to parse the field by distinguishing separate research groups and attempting to identifying specific trends in the data.

The work presented herein fulfills the reporting portion of Subcontract # 0000349956 between Savannah River National Laboratory and the James Martin Center for Nonproliferation Studies.

Introduction

This study examines the structure of scientific networks engaged in research surrounding metal hydrides and solid-state hydrogen storage techniques in Russia. This study leverages network analysis techniques to map the research and organizational entities through an investigation of the pertinent scientific literature. In doing this, the research probes multiple large datasets to identify different characteristics of the scientific networks, including: the primary researchers pursuing each technology and their organizational affiliations; connections that may exist between researchers, research groups, and funding organizations; the materials or processes that are focused on or being used in collaboration with others; and the overall structure of the solid-state hydrogen research network.

Using publicly available data from numerous sources, we collected metadata for roughly 23,000 articles engaging the initial key word list which involved entities from Russia or the Soviet Union over a span of nearly 70 years. This resulted in an extremely large network dataset with significant noise. This initial dataset was examined with a particular focus placed on specific organizations, from which over 400 articles originated. This network contained over 10,000 linkages across different individuals. Scoping down from the original dataset by reframing the search parameters to include only "deuteride" and "tritide" enabled a more precise examination of the types of metals used in the storage process. This included roughly 450 publications and roughly 10,000 connections between different entity types. Using this dataset, the author conducted a multi-modal[1] network analysis to examine the relationships between scholars, institutions, funding, and topic area of research.

This paper is organized as follows: first, we provide a brief overview of the search parameters used in examining the Russian research community; second, the methodology used in the analysis, data collection and organization, network data construction, and network analysis methods to be applied in the analysis section are discussed. Additionally, this section briefly addresses the conceptual framework from which this research proceeds. The ensuing results and analysis section leverage network analysis techniques to model the relational networks over time, assessing the quality of the linkages and their evolution, as well as allowing for the extraction of network metrics that facilitate the quantification of the scientific networks within the Russian solid-state hydrogen storage research community. Finally, the paper will close with general observations from the research.

In this study, we pursued two primary research interests: examine the published R&D literature to (1) attempt to determine which metal hydrides Russian researchers have pursued and (2) make observations on the network structure with regards to two particular organizations. The goal of this line of investigation is to attempt to parse the field (distinguishing separate research groups and attempting to evaluate the relative validity of each) and to evaluate the solid-state hydrogen storage techniques, processes, research, and relative potential across these groups.

This study used open-source bibliographical data to conduct a network analysis of the research being conducted on solid-state hydrogen storage technologies. Mining pertinent metadata from articles and other datasets, the study will construct network models based on relationships of co-authorship, shared institutions, common funding sources, and related research focus to assess progression and potential among the different subgroups. The study will draw upon proven network analysis techniques to model the relational networks, allowing for the extraction of network metrics that facilitate the quantification of scientific networks within the solid-state hydrogen storage and metal hydride communities in Russia.

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[1] Multi-mode network analysis refers to the integration of different types of entities into the same network model. For example, a network model that includes only actors is one-mode, while a model that includes actors and organizations is two-mode. Here, multi-mode is used as we integrate three distinct entity types – actors, organizations, and research areas.

Conceptual Framework

Prior to proceeding into a review of the data sources and methodology, we briefly discuss the conceptual framework that guides this research to better frame the approach and intended output. Fundamentally, our approach is attempting to probe the knowledge infrastructure surrounding solid-state hydrogen storage in Russia to better understand and assess the development and current capacity of tacit knowledge. A workable definition of tacit knowledge suitable for our purposes here is the knowledge that is difficult to acquire, transfer, and develop, and is advanced through experience and development, rather than through explicit means. Hence, tacit knowledge must be learned through trial and error to fully grasp the eccentricities of the information and processes. This trial and error process directly involves scientific process, particular equipment, other scientists and engineers (experienced or in learning groups), and institutional resources. As such, this process of tacit knowledge development can be thought of as repeated interaction between actors in a network. Institutions, funders, and topics are also pertinent here as they provide further structure and hierarchy to the network, facilitating knowledge transmission without directly transmitting it themselves. In other research by the author, it is posited that the network structure and role of institutions in the network can have a significant impact on the scientific community, and thus the ability of a state to proliferate.

As has been noted, "knowledge is fruit of the circulation and interpretation of information, cumulative experience and cognition."[2] Relationships are critical to attaining tacit knowledge, as its development is inherently a social and interactive process.[3] These relationships within networks enable us to understand who the key actors are in furthering tacit knowledge development in the study of tritium and its production.[4] Additionally, the structure of the network, conceptualized in network analysis as lasting patterns of relations among actors, is important, as it allows inferences to be drawn about the expected action by, and capacity of, clusters of individuals.[5] In this context, this research focuses on the relationships as the key to the learning processes that enable tacit knowledge acquisition, and they are the starting point for this framework.

Network analysis enables an examination of the structural relationships between social entities. It is through these relationships that one can identify tacit knowledge development, as shown through repeated interactions of scientists, engineers, and other actors who engage in scientific exploration. As tacit knowledge is developed and transferred through repeated and substantial interaction, one can expect networks in which scientists and engineers are heavily interacting with one another to be more efficient in developing tacit knowledge than others. It is also possible, through the examination of these networks, to identify evolving research foci, emergent communities, or key organizing institutions. While institutions can be critical to organizing research, they can also have adverse effects. Institutions, such as universities, government agencies, or laboratories, can serve a role by facilitating a "shared knowledge space," by which resources and knowledge are able to be transferred more efficiently (think of sharing an office space with someone), but does not inherently increase the level of tacit knowledge in the system. That said, institutions play a key role in providing structure and hierarchy to the network. In the following analysis, we will be able to observe particular power centers in tritium research, and to whom those power centers are connected.

[2] Glückler, J. "Knowledge, Networks and Space: Connectivity and the Problem of Non-Interactive Learning," *Regional Studies*. (47:6, 2013), pg. 881.

[3] Borgatti S. P. and Cross R. A relational view of information seeking and learning in social networks," *Management Science*. (2003) 432–445.

[4] Glückler, 885.

[5] Ibid.

Data Sources

This research utilized open-source scientific literature from a variety of sources. Bibliographical data from the Web of Science, the International Atomic Energy Agency's International Nuclear Information System, Scopus, Google Scholar, and other bibliographical indexes were collected. Data were collected based upon an ontology of scientific terminology provided by technical experts at Savannah River National Laboratory (SRNL) that are pertinent to solid-state hydrogen storage. This initial list of search terms was utilized to pull data from the various sources listed above. The search terms used in the preliminary data collection phase are shown in Table 1 in both English and Russian.

Table 1: Search Terms

Search Terms	
English	**Russian**
boron	бор
chromium	хром
deuterium	дейтерий
diffuser	диффузор
erbium	эрбий
getter	добытчик
He-3 separation	Разделение He-3
Helium	гелий
helium aging	старение гелия
helium-3	гелий-3
hydride	гидрид
hydrogen	водород
hydrogen absorption	поглощение водорода
hydrogen desorption	десорбция водорода
hydrogen isotopes	изотопы водорода
hydrogen storage	хранение водорода
isotherm	изотерма
isotherm measurement	измерение изотермы
isotope separation	разделение изотопов
LaNi5	LaNi5
lanthanum-nickel	лантан-никель
lanthanum-nickel-aluminum	лантан-никель-алюминий
metal hydride	гидрид металла
palladium	палладий
permeator	мембранный разделитель
release of helium	высвобождение гелия
release of tritium	высвобождение трития
Separation	разделение
tellurium	теллур
titanium	титан
tritium separation	разделение трития
tritium	тритий
uranium	уран

The resulting dataset using these key terms included a significant amount of noise and false positives. While we attempted to scope down by focusing on particular areas of research (i.e., physics or inorganic chemistry), the remaining publications still remained significantly opaque. Some analysis was conducted on two specific organizations within the dataset, which will be presented later in this paper, but a refocusing of the research was also undertaken.

Following discussions with SRNL researchers after review of the initial dataset, a new search was conducted on the English and Russian translations for "deuteride" and "tritide," with an emphasis on metals and metal alloys used in solid-state hydrogen storage. This shift significantly reduced the size and noise of the dataset to a manageable level. While the first data collection phase enabled an organizational focus, the refocused dataset allowed for a more attentive examination of the materials engaged by Russian scientists.

In past research using this approach, the data were cleaned to focus on collaborations that did not include large project teams. It is argued that larger project teams, typically of more than just a few individuals, is not efficient for knowledge transfer across all entities in the team. Rather, in these situations, individuals on the project team will typically focus on different components of the research rather than having visibility into all stages of the processes and materials used. Only extremely large teams of participating authors were removed from the analysis. It is worth noting that in the case of reconfigured search parameters, the number of large contributing research teams was minimal.

Methodology

This research will draw upon network theories and network analysis to distill the partnerships and interactions that highlight research into solid-state hydrogen storage in Russia. Using network analysis techniques and statistics, the research will attempt to distill the various groups, subgroups, and materials used in Russian research.

From the bibliographical data on each document, an interaction matrix was created by which all components contributing to a paper were broken down and connections classified by one of three categories, as was discussed earlier. These include agents (authors on papers), organizations (associative institutions), and funders (funding institutions). Additionally, the search terms form another network in which each author engaged a particular subject area. These ties were added to better assess the structure of each research area.

Each connection between entities was assigned a value of 1, with the software compiling each interaction observed in the specified time period. As such, the more interactions an entity had with another entity over the course of a defined period, the stronger the relational connection. Ties between agents and ties between institutions or materials were both classified as undirected, meaning that it was not one entity initiating the relationship, but rather a mutually agreed to arrangement in which both entities benefited equally. Relationships between agents and institutions were considered directional, with the link flowing from agent to institution. This was specified this way as agents (authors) have agency in tacit knowledge relationships, while institutions do not.

With the network data established, the author conducted a variety of network analysis techniques to assess the structure of the groups at different levels and across different entities. Network statistics of different agents and institutions were also collected and presented. As this research does not seek to establish a causal relationship, the following presents more of a survey of the networks that are of interest.

Network Statistics

Prior to presentation of the summary statistics and results, it is worth noting several terms with regards to network statistics that will be presented. There are two broad classifications for these terms. The first is network-level, which provides data on the characteristics of the network (or sub-networks) as a whole. This will help to inform as to what the overall capacity and emphasis of the network is. The second is actor- level, which provides details as to the standing of particular individuals or organizations within the network (or sub-networks).[6] These statistics provide insight into who the important particular entities are in preforming particular functions, such as transmitting information between various sub-groups or being well-connected to entities which are above their status in the network. The following provides a short definition of some of the terms that may be used throughout the remainder of the paper.

[6] Given the refocus of the research onto the materials used rather than individuals, the network statistics related to the actor level which are presented further in this research are limited.

Network-Level

Density: The number of links divided by the number of possible links not including self-reference. For large data network analyses, this figure will be extremely small, as most entities in the network will have interaction with only a minor subset of other entities. It is presented here only to help inform the evolving characteristic of the networks.

Network Centralization (total): Fundamentally, a composite of all total degree centrality scores for each entity within a single network (agents, organizations, search). Again, this provides insight into the overall structure of the network and to what extent it is interlinked.

Clustering Coefficient: Measures the degree of clustering in a network by averaging the clustering coefficient of each node. The clustering coefficient gives a sense of the local characteristics of the network. A higher clustering coefficient is indicative of closely linked sub-groups, while a low clustering coefficient suggests that sub-groups are not highly interactive.

Actor-Level

Total Degree Centrality: The normalized sum of a node's in links and out links. Often referred to as the measure of “in the know” as it captures total in and out linkages for an entity. Individuals or organizations who are "in the know" are those who are linked to many others and so, by virtue of their position, have access to many different entities.

Betweenness Centrality: Across all node pairs that have a shortest path containing a particular entity, betweenness centrality is the percentage that pass through that entity. This measure identifies nodes that connect disconnected groups, like a go between, broken, or gatekeeper between entities. This statistic has been critical in many sociological, organizational, and terrorist studies. For the purposes of this paper, an individual with a high between score could be thought of serving, potentially, as a systems engineering role, in that they engage with many different groups or areas of research.

Eigenvector Centrality: Reflects an entity’s connections to well-connected entities. For example, if I have only a few connections, but all of them are to critical nodes in the network, I would receive a high eigenvector centrality score. Additionally, eigenvector centrality per component may be used. This measure captures the score for each entity of the network individually, scales the values according to the number of nodes in the network, and then combines the values into a single measure.

Bonacich Power: Actor’s centrality is equal to a function of the centrality of they are connected to. Thus, actors who are tied to very central actors should have higher centrality (or prestige) than those who are not.

Clique Count: The number of distinct sub-structures, defined as a set of nodes where every node is connected to every other node, to which each node belongs.

Triad Count: A triad is a relationship amongst three nodes. This measure captures the number of triads in which a particular node is at the center (connecting two other nodes).

Capability: Detects entities with high or low degree relative to other entities. The formula discounts for the fact that most agents have some connections and assumes that there is a general discount to having large numbers of connection.

Formatting Note

A brief note on formatting is necessary on the network graphs presented. A standardized color scheme was applied to all networks to ease interpretation across different graphics. All entities, or nodes, are represented with small shapes. Agents (authors) are red circles, organizations are blue squares, and research areas are black triangles. Links between two entities have similar coloring, with agents as a lighter red, organizations a lighter blue, and research areas grey. Organizational connections indicated funding are in green. In most cases, the width of connections between two nodes is sized based on the strength of the relationship, to easily distinguish which two nodes are interacting with great frequency from those with limited interaction. Nodes will also be sized, in most graphs, according to a network measure to identify critical nodes in the network. The statistical measure will often be total degree centrality.

Most graphs are presented here using a Multidimensional Scaling (MDS) technique. MDS provides a visual representation of the pattern of similarities among the nodes in the network. MDS plots nodes in the network in such a way that those nodes that are structurally similar to each other are placed near each other on the map, and those nodes that are perceived to be very different from each other are placed far away from each other on the map. The result of which is to promote clustering in the network graphs for those entities that are closely related, while distributing unlike groups elsewhere in the diagram.

Finally, to identify particular clustering and structural equivalence, two cluster analysis techniques were used to detect collaborative groups. First is to partition network data by splitting blocks based upon the convergence of iterated correlations, known as CONCOR. Given an adjacency matrix, or a set of adjacency matrices for different relations, a correlation matrix can be formed. This matrix is then used to split the data into two blocks such that members of the same block are positively correlated, whereas members of different blocks are negatively correlated. Second, Newman clustering is a hierarchical method used to detect communities in complex systems. It is used to detect communities by progressively removing edges from the original network, with the links remaining being the related communities. Both of these approaches allow for identification of communities across different entity types, research areas, and individual collaborations.

Results and Analysis

The following section will present the results of the research in three parts. First, a brief review of summary statistics will be presented to demonstrate scope and display other indicators present in the data. Next, the network structure of research and technical focus for two particular organizations will be examined. Finally, a network analysis of the narrowed dataset is conducted to concentrate on the materials used by Russian scientists.

Summary Statistics

At the start, it is useful to break down the networks into some very high-level summary statistics to better assess the structure and content of the network. Rather than touch upon the larger, noisier dataset, the following will focus solely upon the materials and research areas found in the smaller datasets targeted at examining the “deuteride” and “tritide” search parameters. Table 2 shows the number of papers in which specific materials were identified and the interactions present between each material and other materials in the same paper. For example, research results presented in a paper that contain work in both alloys and nickel would be an interaction for each keyword.

Table 2: Search Terms: Paper Count and Total Interactions

Material Keyword	Paper Count	Interactions with Other Material Keywords
alloy	52	154
aluminum	17	43
antimony	1	2
barium	1	6
beryllium	10	13
ceramic	2	4
cerium	1	4
cesium	6	26
chromium	16	66
cobalt	9	31
dysprosium	1	5
erbium	7	25
gadolinium	3	15
gallium	1	2
hafnium	12	32
holmium	2	15
iridium	1	3
iron	30	99
lanthanum	7	32
lithium	74	100
magnesium	4	17
manganese	5	19
molybdenum	5	28
nickel	33	107
niobium	4	12
palladium	39	99
platinum	14	26
potassium	1	1
praseodymium	1	3
rhodium	2	11
ruthenium	2	4
samarium	1	5
scandium	2	10
stainless	7	31
strontium	1	6
tantalum	2	4
terbium	6	26
thorium	2	7
thulium	1	2
titanium	69	152
vanadium	34	95
ytterbium	1	2
yttrium	4	18
zinc	2	6
zirconium	54	150

While not presented here, Table S1 includes the network statistics for each of the metals included in the above table to provide further insight into the network position and stature of the metal in the research networks.

In looking at the results of the narrowed search parameters, the number of papers that resulted from data collection and the subsequent links into each that could be discerned are listed in Table 3. Immediately noticeable is the difference in interactions present between the two search terms. This can be attributed to the variation in quality of the data from the different sources and the age of the research papers (more recently published papers generally have better metadata). While an automated classification system was used to identify all metals and pertinent materials present, a manual review process was also conducted to ensure that the data was consistently classified and included all metals mentioned in the paper descriptive metadata.

Table 3: Papers and Interactions with Search Terms

Material Keyword	Paper Count	Interactions with Other Material Keywords
deuteride	301	484
tritide	149	75

Table 4 presents summary network statistics for the two distinct networks derived from the "deuteride" and "tritide" data collection process (overlap of the networks is not included here given the different entity types). This table highlights the varied characteristics of the networks. For example, given the small number of nodes in the network and similarity in research, the material network is more consolidated and ties are more redundant. Also expected is that the network composed of individuals is more disperse and more fragmented. Interestingly, the average distance is relatively on par for the two networks and the degree in which the networks are clustered. This is likely due to the similar general area of research shared by the individuals in the network.

Table 4: Summary Network Statistics

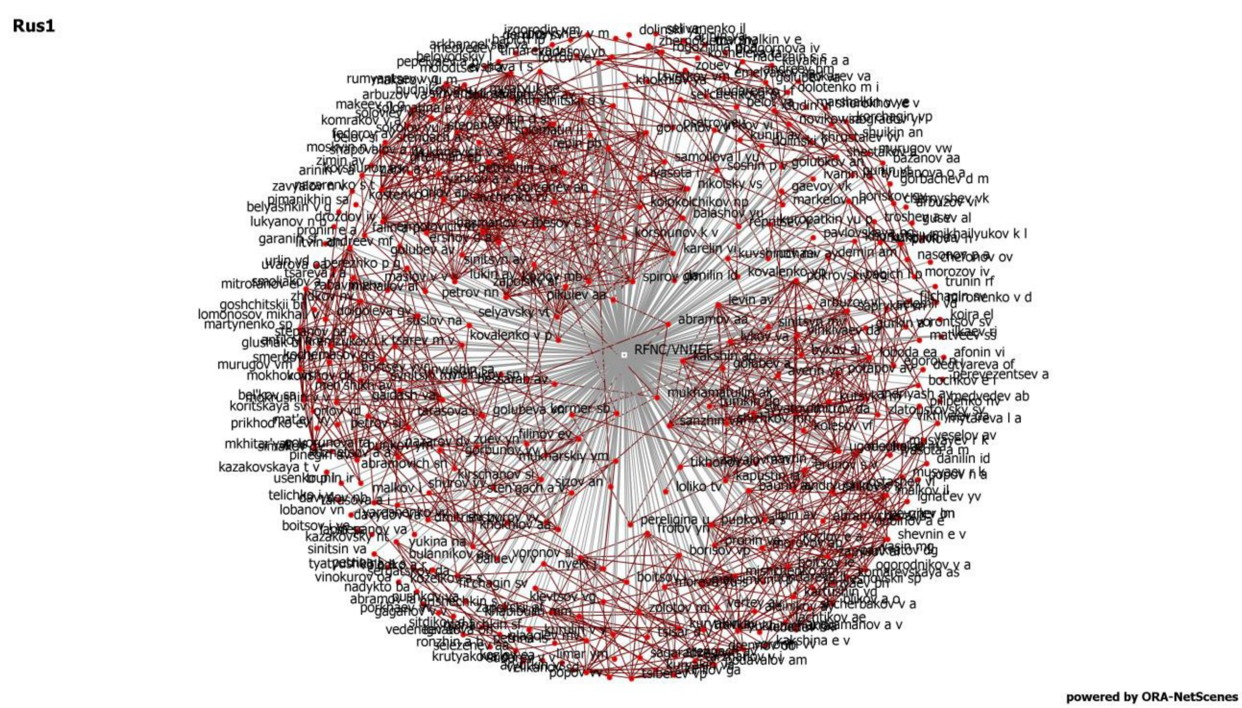
Measure	Material Network	Individual Network
Average Distance	3.59	2.69
Average Speed	0.28	0.37
Clustering Coefficient	0.39	0.42
Density	0.120	0.004
Diameter	2592	25852
Diameter Reachable	21	27
Diffusion	0.31	0.01
Link Count	271	4560
Link Sum	1048	7348
Fragmentation	0.00	0.89
Global Efficiency	0.46	0.03
Node Count	48	1124
Row Redundancy	0.46	0.01
Span Of Control	24.37	8.08
Transitivity	0.54	0.72

Organizational Focus

At the start of this study, the broad set of key terms provided was augmented with a list of organizations that were of particular interest given their long history of research in this area. In the past, similar research has focused on individuals and organizational discovery. For the purposes of this research, however, the focus is placed upon the structure of research emerging from two particular organizations in order to assess the structure, size, and interaction in these communities.

The following section presents the network graphs for those associated with either Russian Federal Nuclear Center (also referred to as VNIIEF or RFNC) or A.A. Bochvar High-Technology Scientific Research Institute for Inorganic Materials (VNIINM). The graphics are for the first and second degree connections surrounding each organization.[7] The CONCOR grouping coloring (indicated in title of graphic) in files is used to identify those groups that are structurally similar, whereas the Newman clustering (indicated in the title of graphic) attempts to identify local communities within a network. The primary objective of these graphics is to illustrate the breadth of the networks, unique clustering patterns, and general organization of individuals associated with each.

Figure 1: RFNC 1st Degree Network



[7] A first degree network are those with direct connection with the organization. A second degree network contains the links to those with connections to the organization.

Figure 2: VNIINM 1st Degree Network

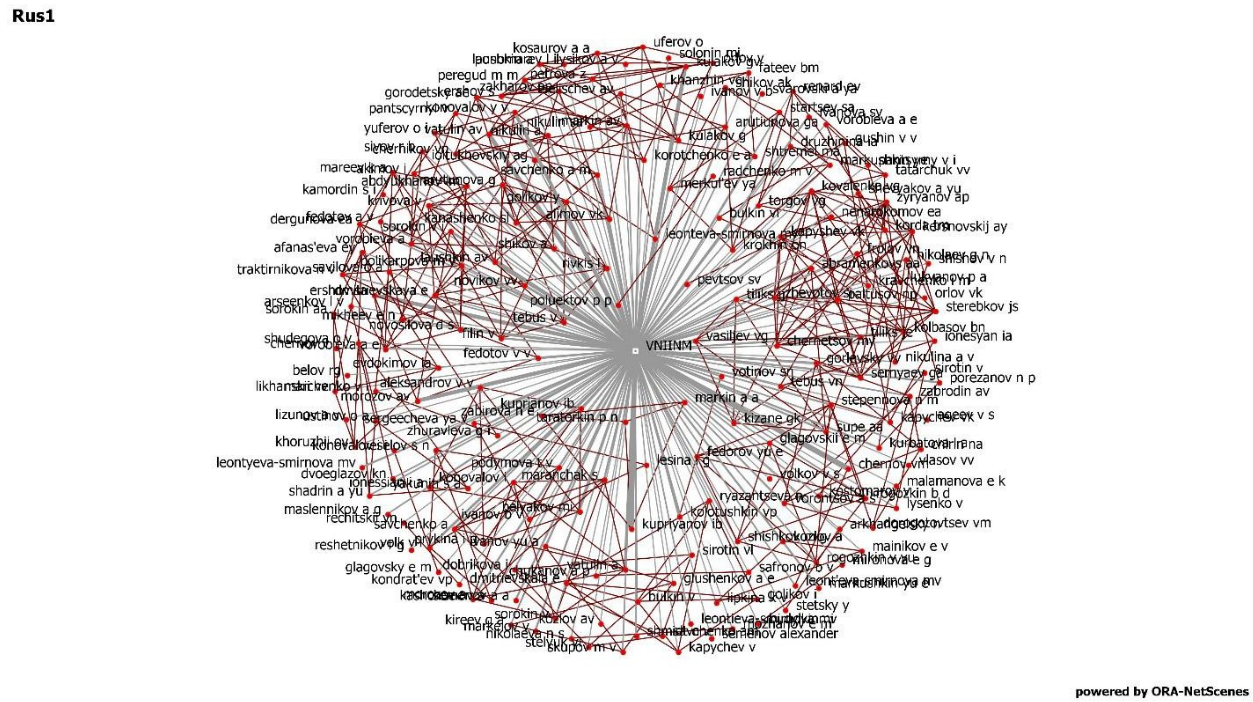


Figure 3: RFNC 2nd Degree Network

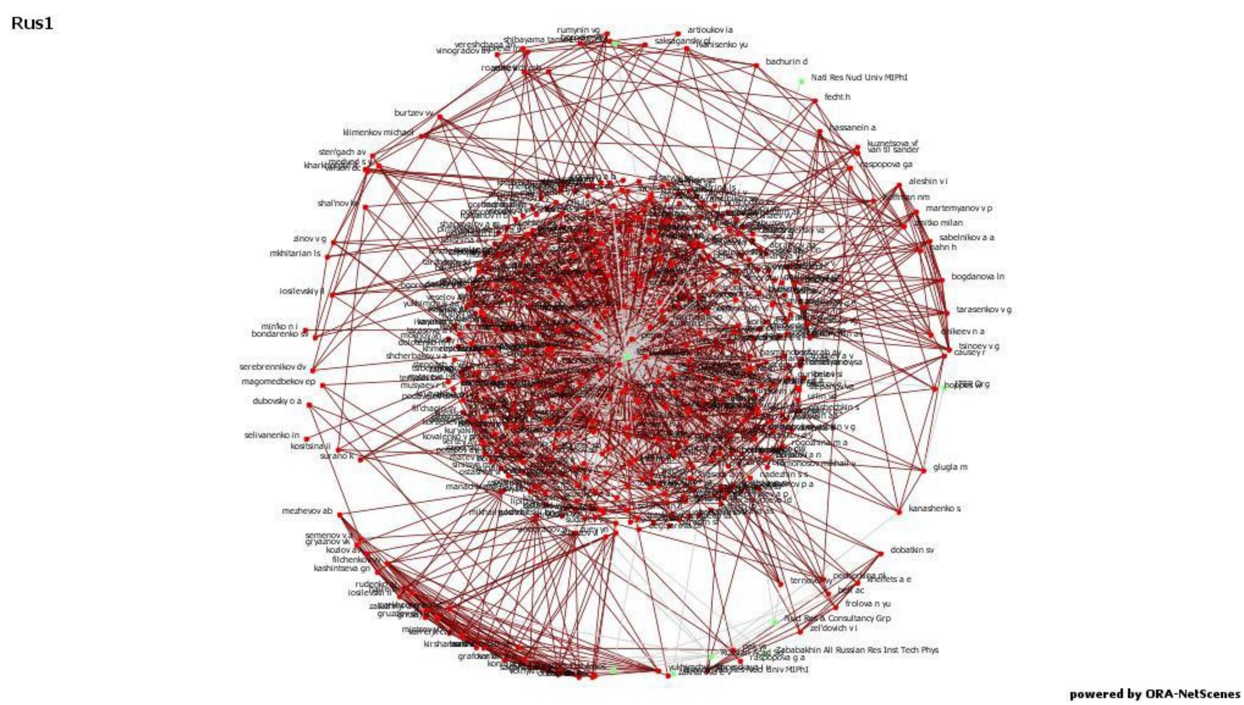


Figure 4: VNIINM 2nd Degree Network

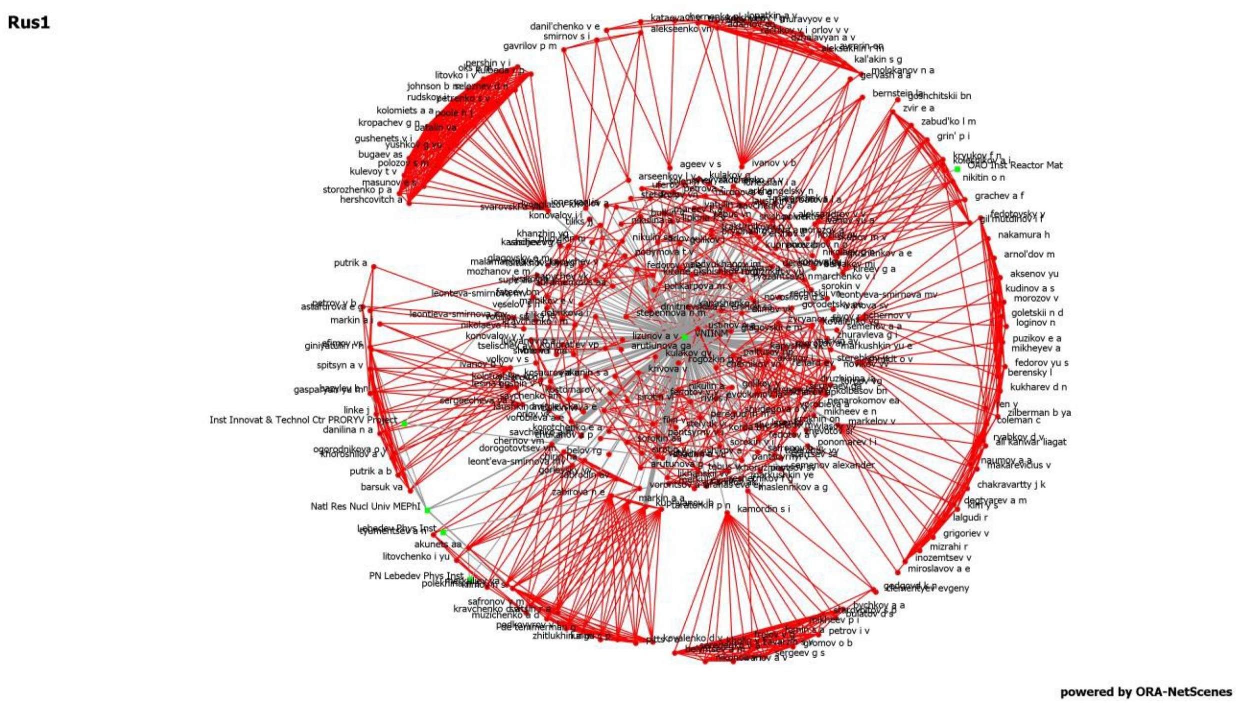


Figure 5: RFNC 1st Degree Network CONCOR Grouping

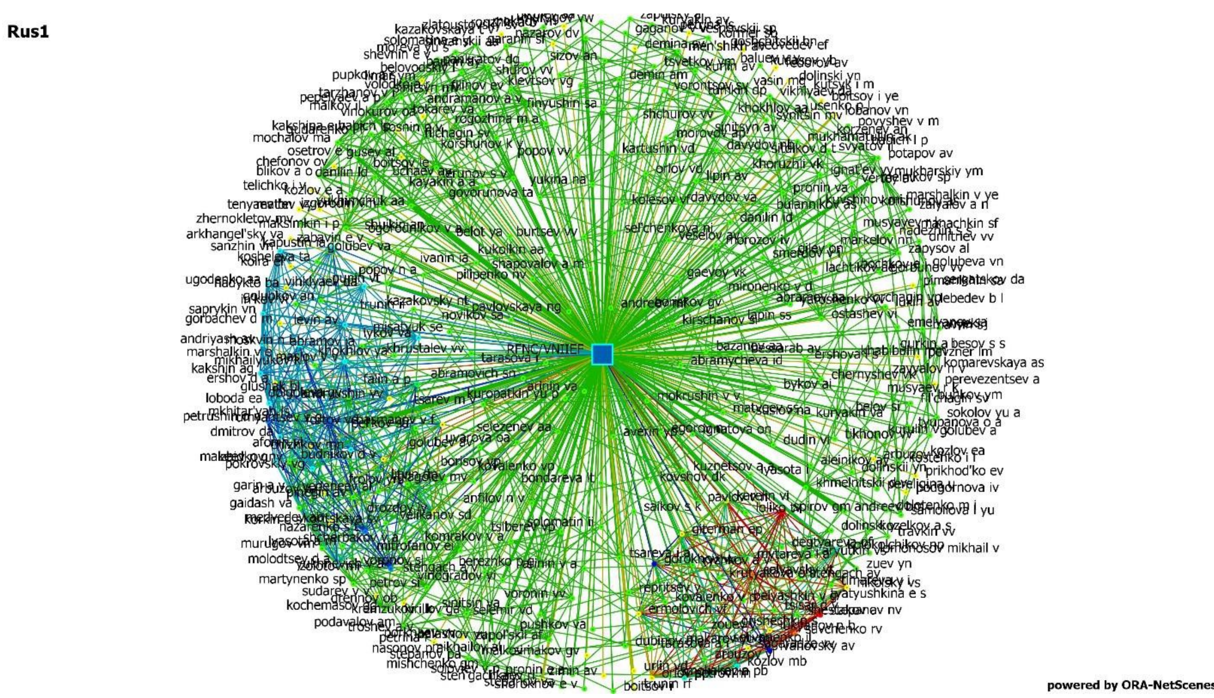


Figure 6: RFNC 1st Degree Network with Newman Clustering

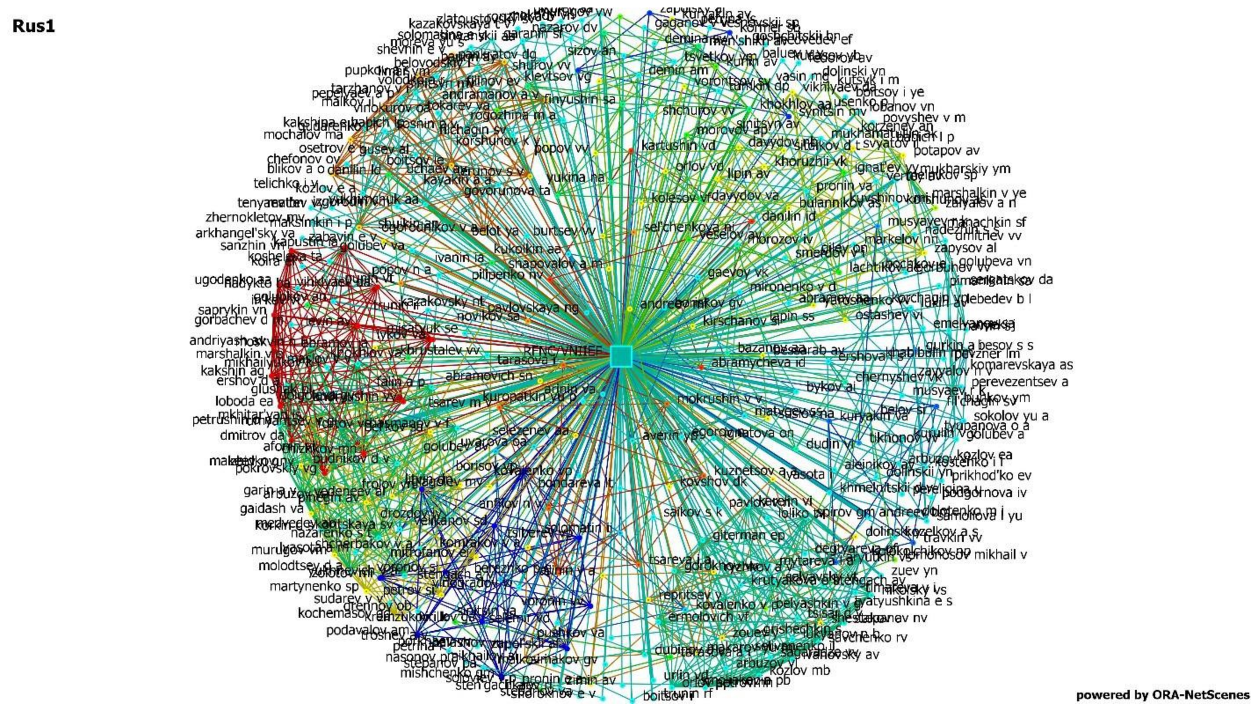


Figure 7: VNIINM 1st Degree Network with CONCOR Grouping

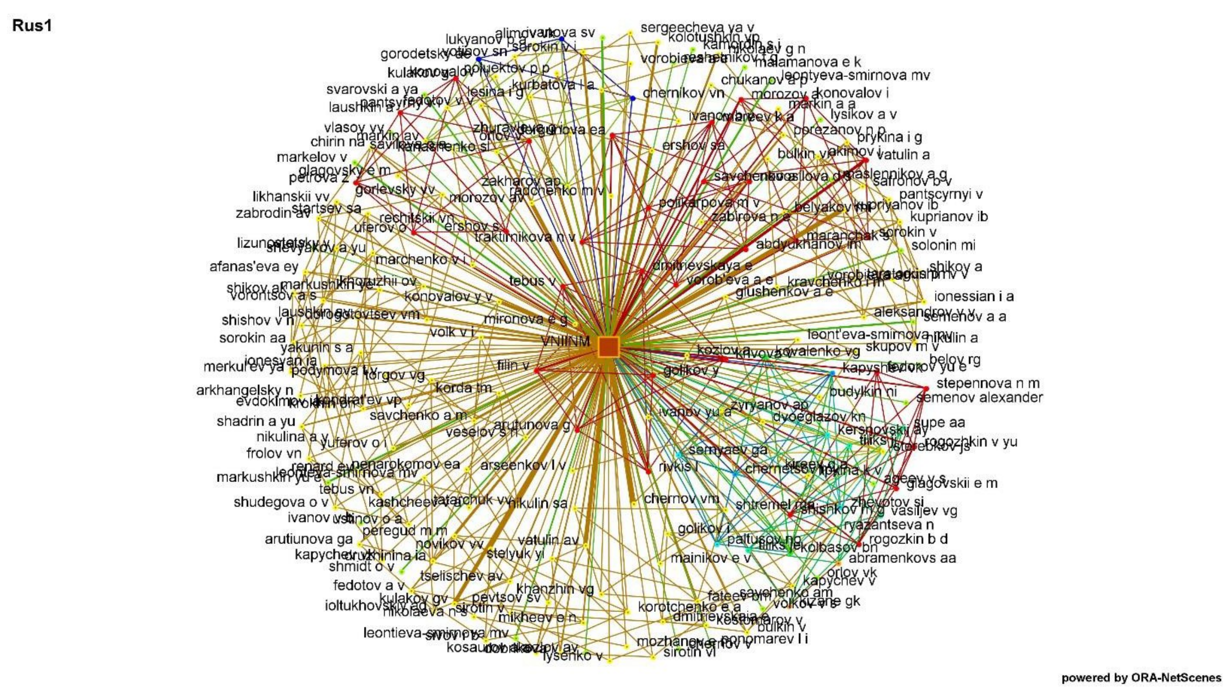


Figure 8: VNIINM 1st Degree Network with Newman Clustering

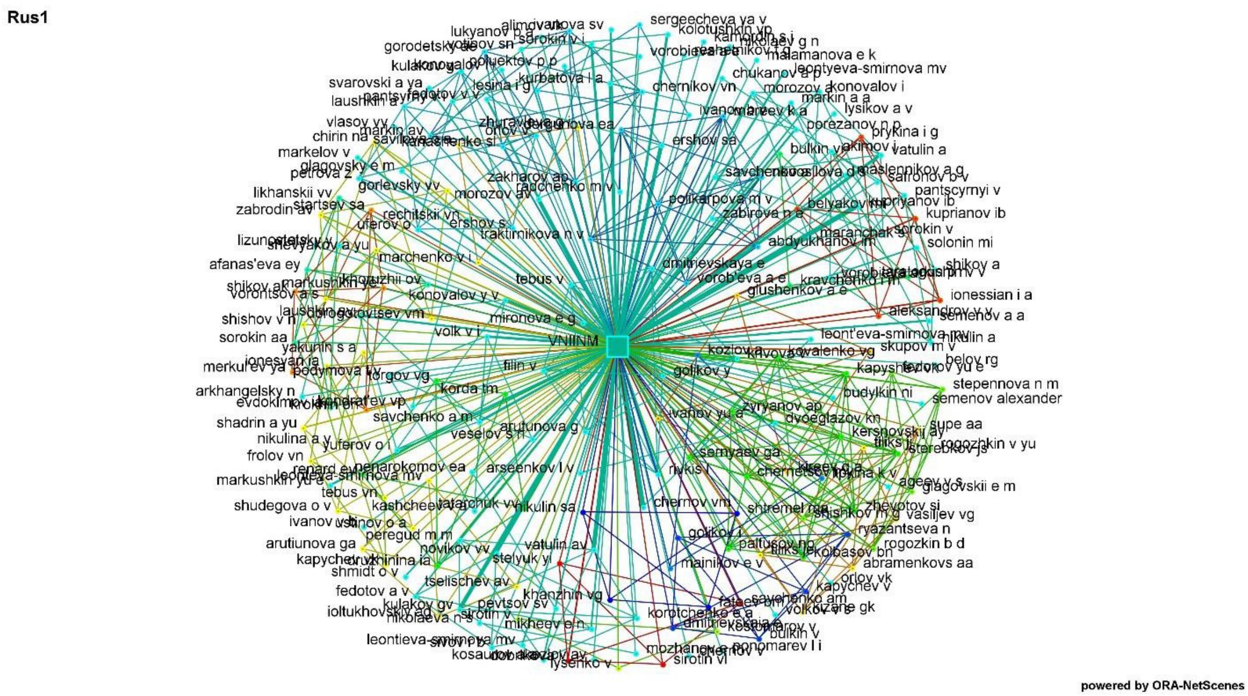


Figure 9: RFNC 2nd Degree CONCOR Grouping

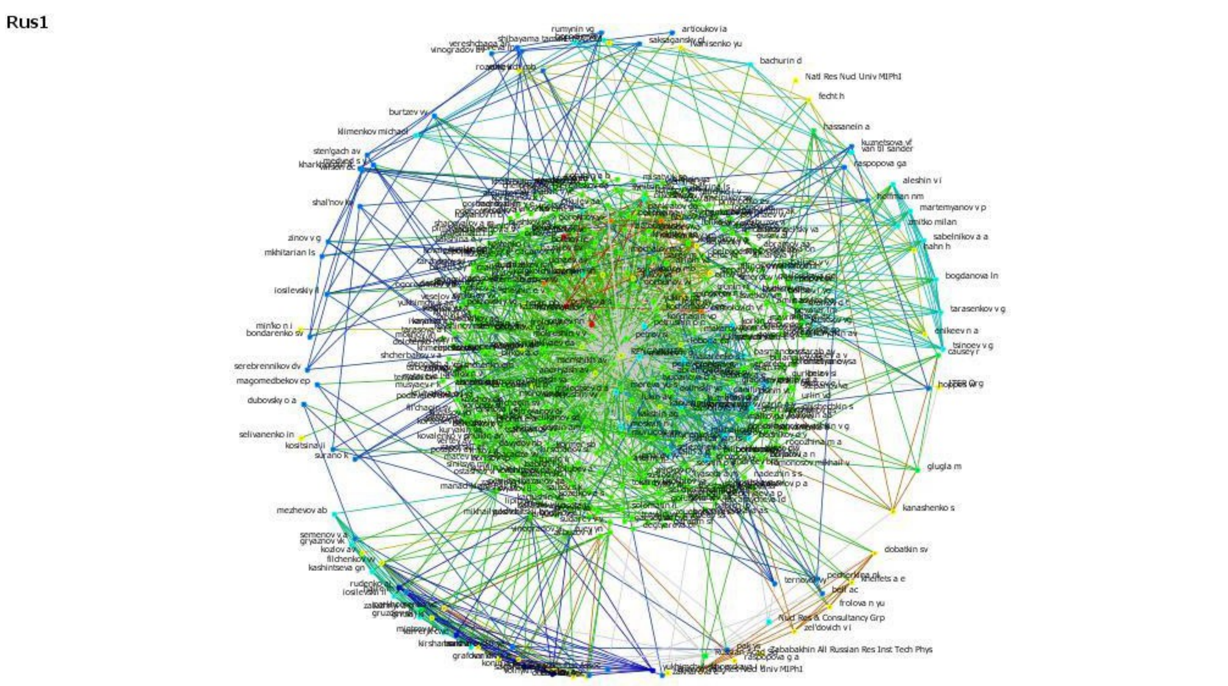


Figure 10: RFNC 2nd Degree Newman Clustering

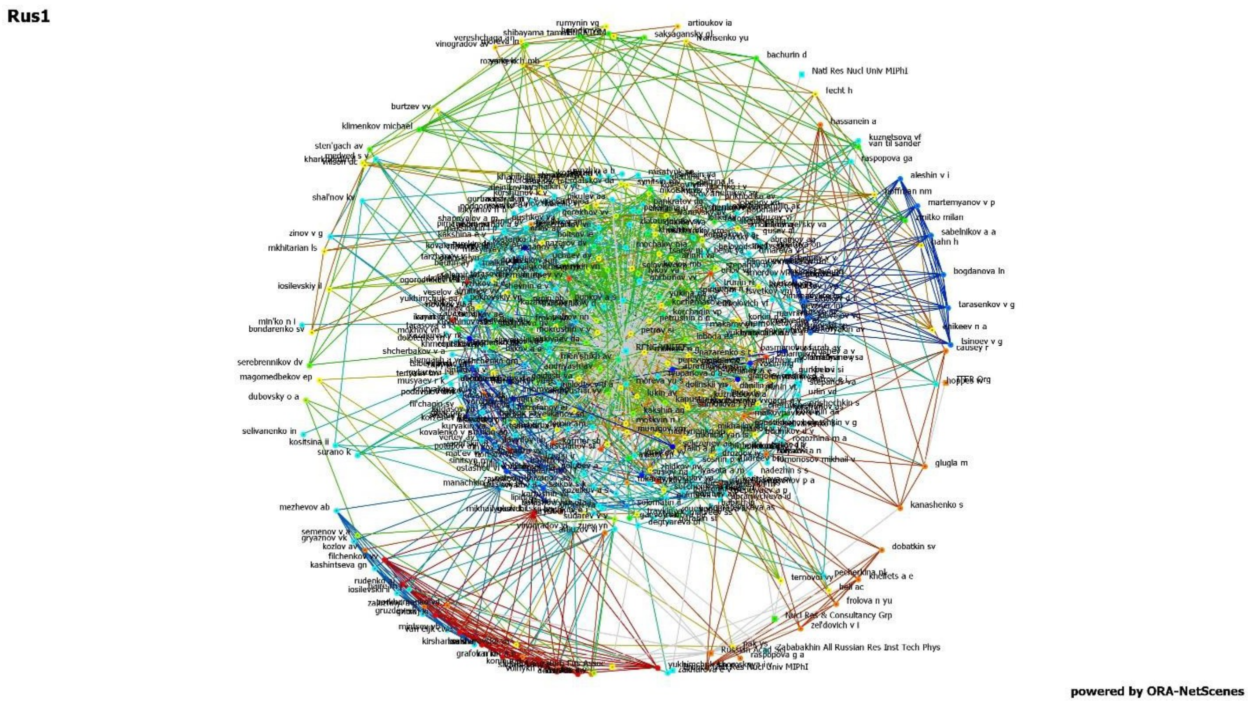


Figure 11: VNIINM 2nd Degree Network with Newman Clustering

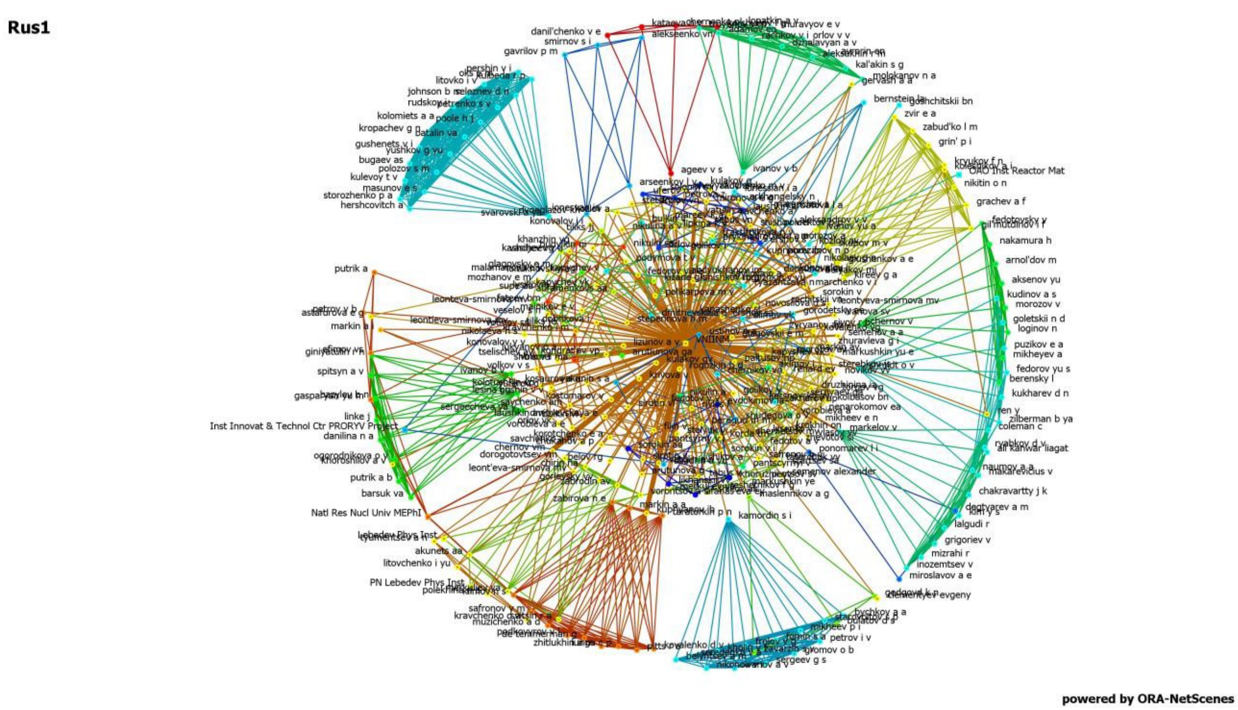
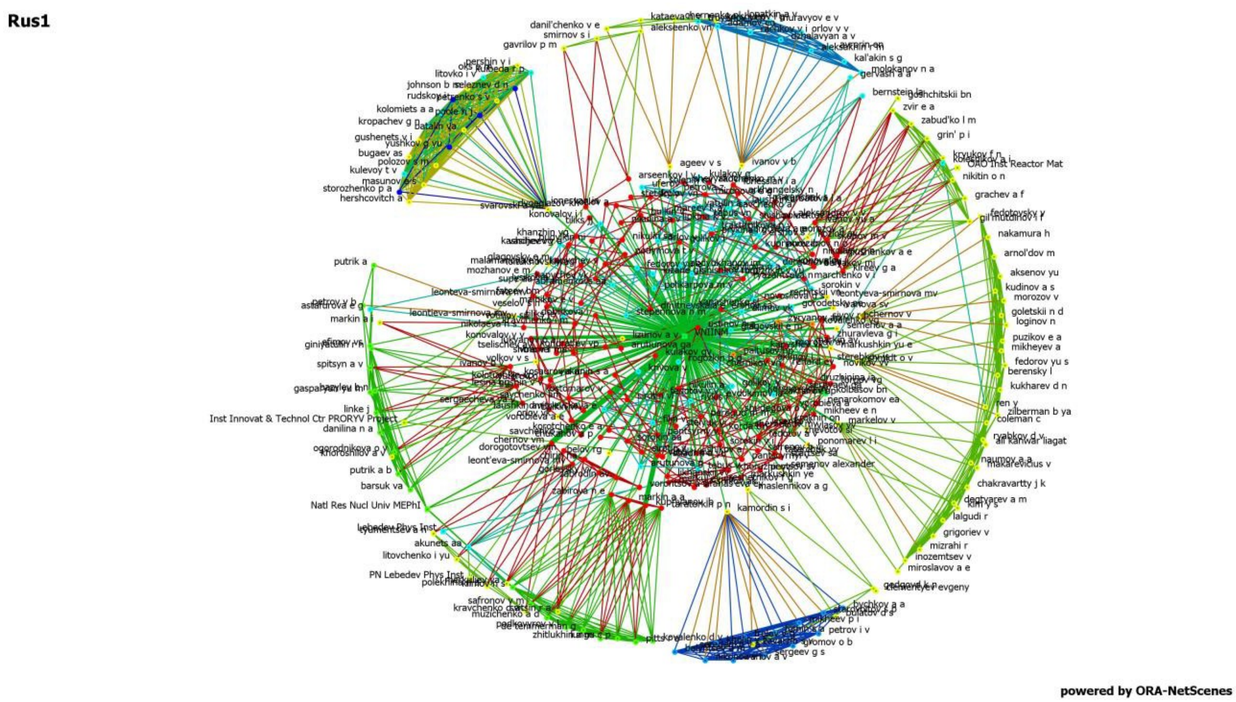


Figure 12: VNIINM 2nd Degree Network with CONCOR Grouping



In addition to considering the networks for each organization separately, Figures 13 and 14 illustrate the aggregate networks for the two groups, showing cross-organizational efforts both in terms of all ties and strong ties, as well as interaction with particular technical terms. Both figures show connections between individuals in red and the connection with technical terms (materials, processes, equipment) in blue. As expected, there is a general convalescing around particular processes and materials in both figures. However, it is interesting the extent to which a dominant core does arise in each network graph with peripheral sub-groups with limited connectivity.

Figure 13: Technical Term Network with All Ties

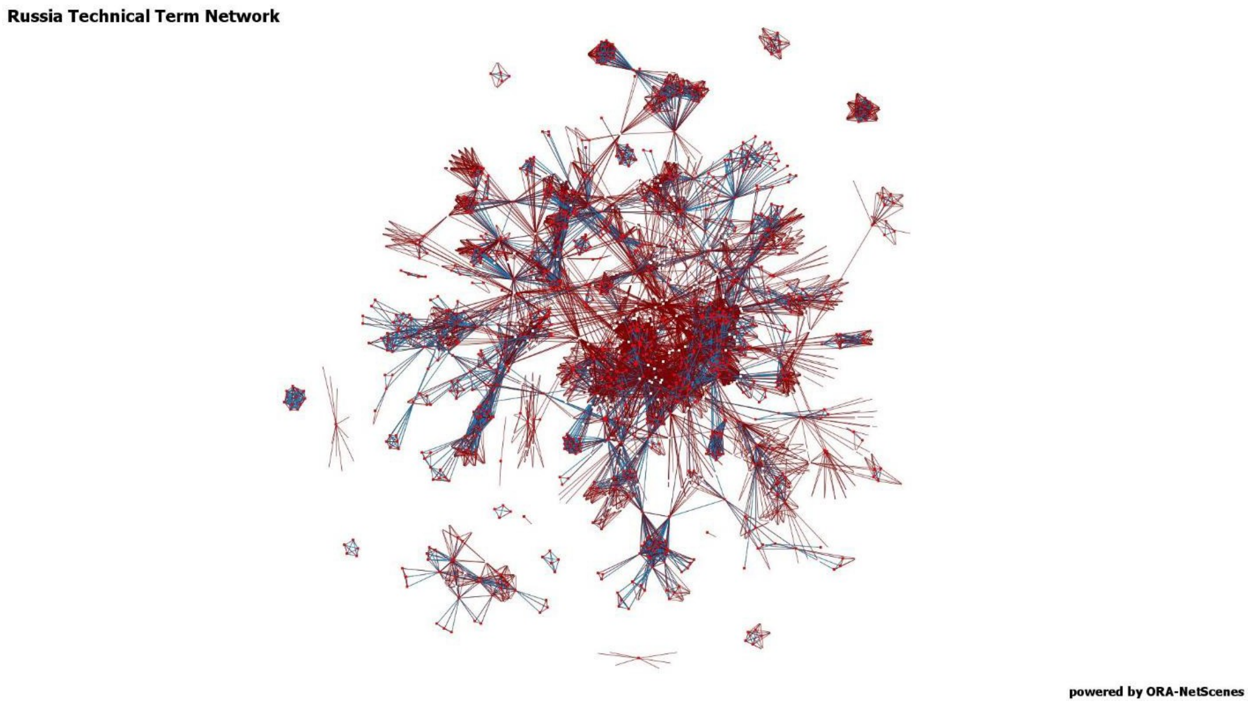
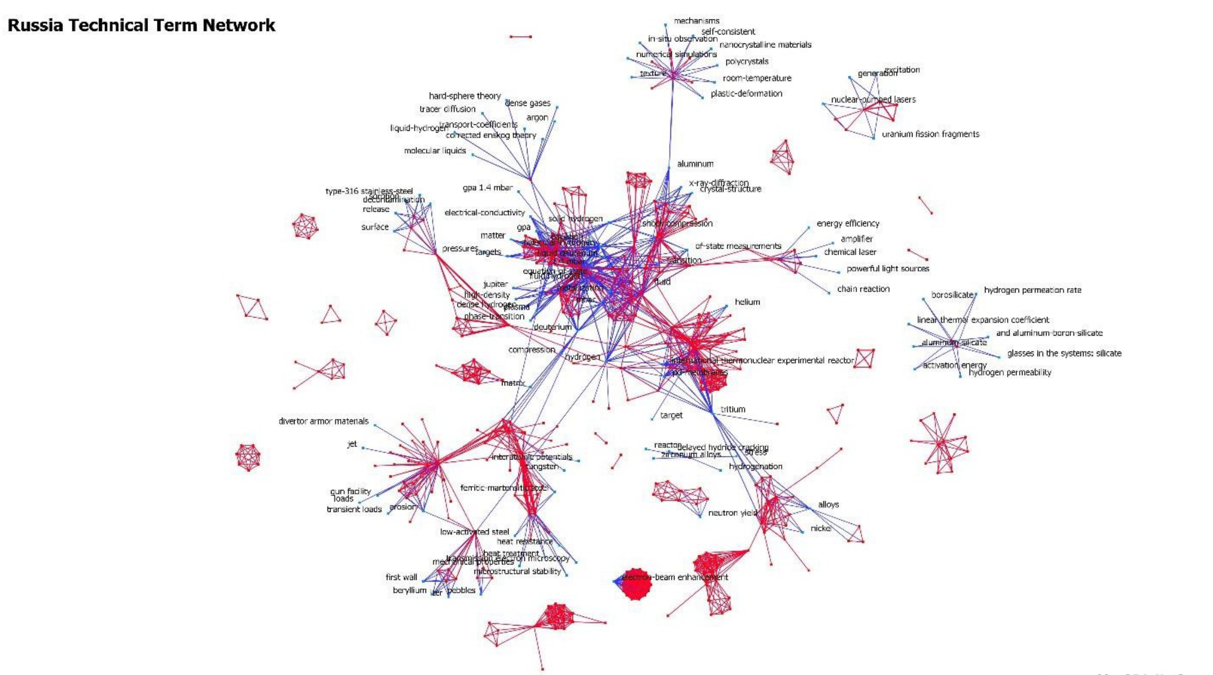


Figure 14: Technical Term Network of Strong Connections



Material Focus

Pivoting from the larger search parameters to refocus more narrowly on research involving "tritide" and "deuteride," the next section examines the interaction of particular metals and other materials in the research. The objective here is to highlight the different communities which surround each type of material and where particular materials intersect in the research.

The next ten network graphics show the links between individuals and materials, as well as materials and other materials. Connections and nodes in red are those that engage an individual, whereas those in black represent metals and other materials and the connections between materials. Each is organized such that similarly connected objects (those with many shared connections) are placed closer together in the network chart. As such, denser grouping of red and black nodes indicates significant engagement between the entities rather than a single observation.

Each paper was classified as resulting from either the "deuteride" or "tritide" search parameter. As such, a connection engaging either of these terms is present in all graphics.

Figure 15: 1st Degree Network of Alloy

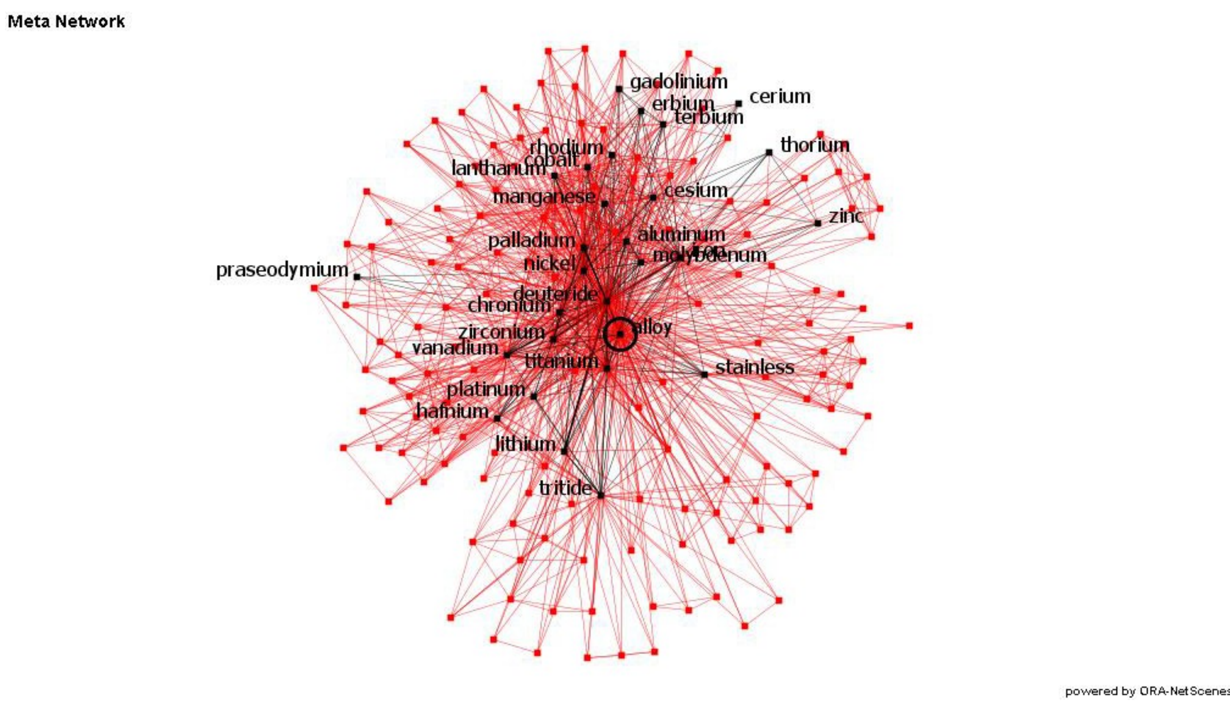


Figure 16: 1st Degree Network of Zirconium

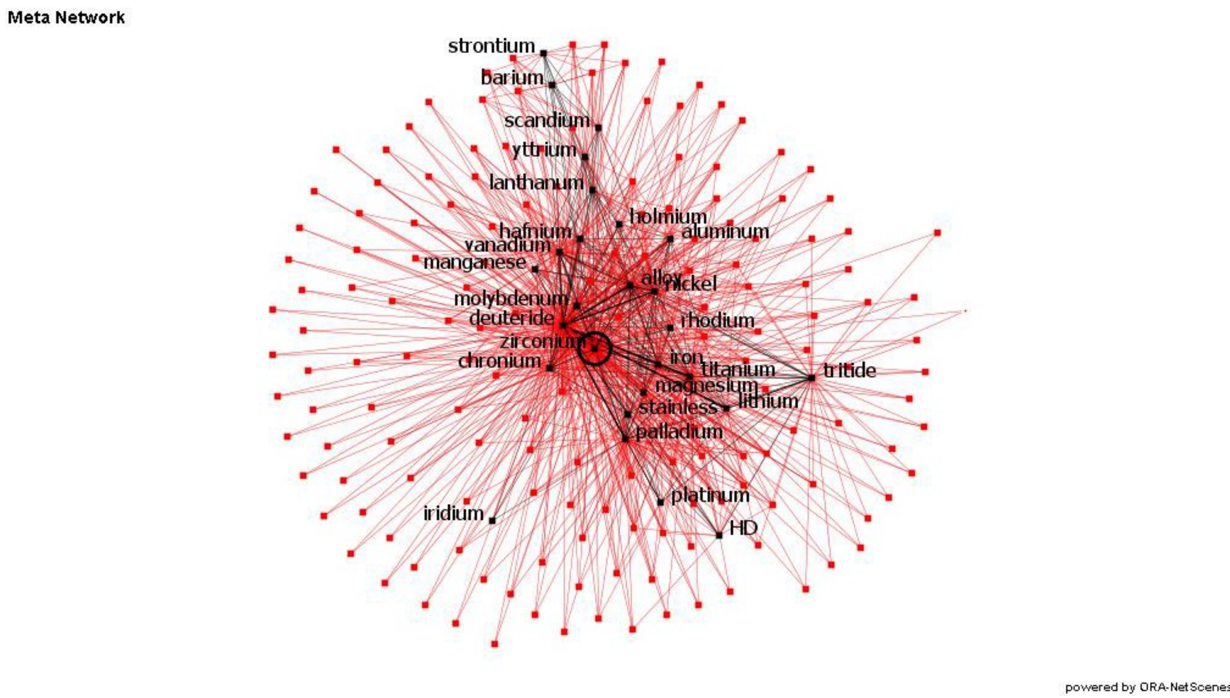


Figure 17: 1st Degree Network of Iron

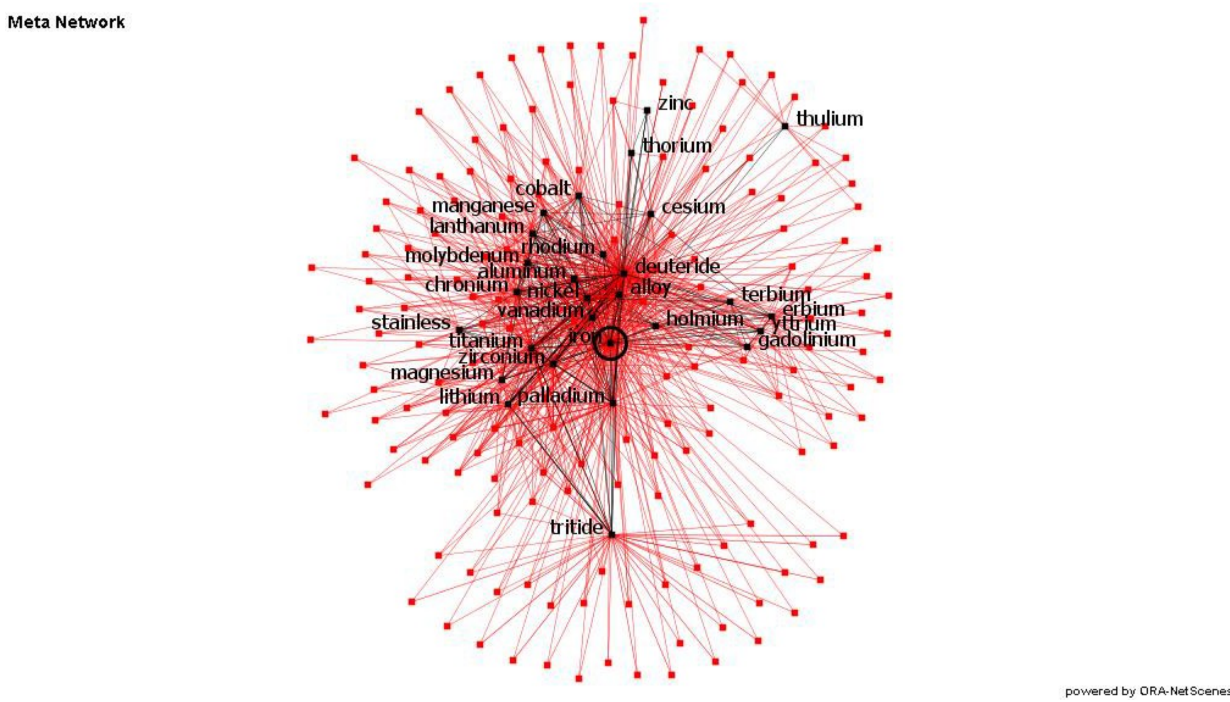


Figure 18: 1st Degree Network of Nickel

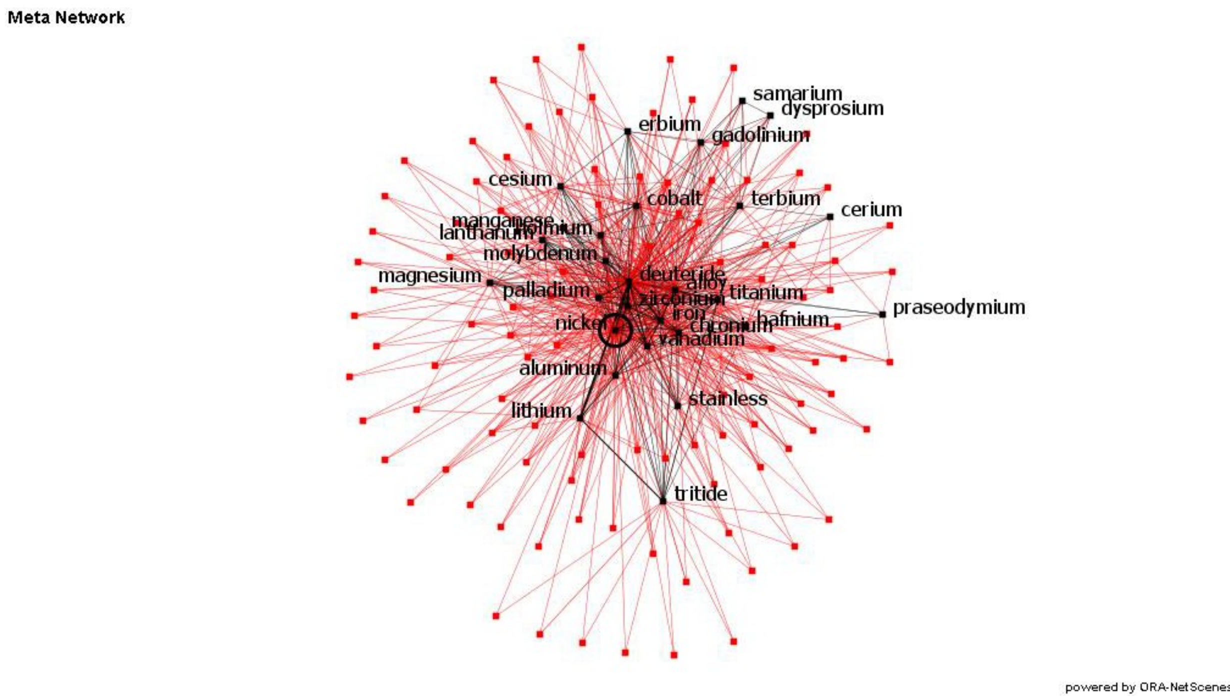


Figure 19: 1st Degree Network of Palladium

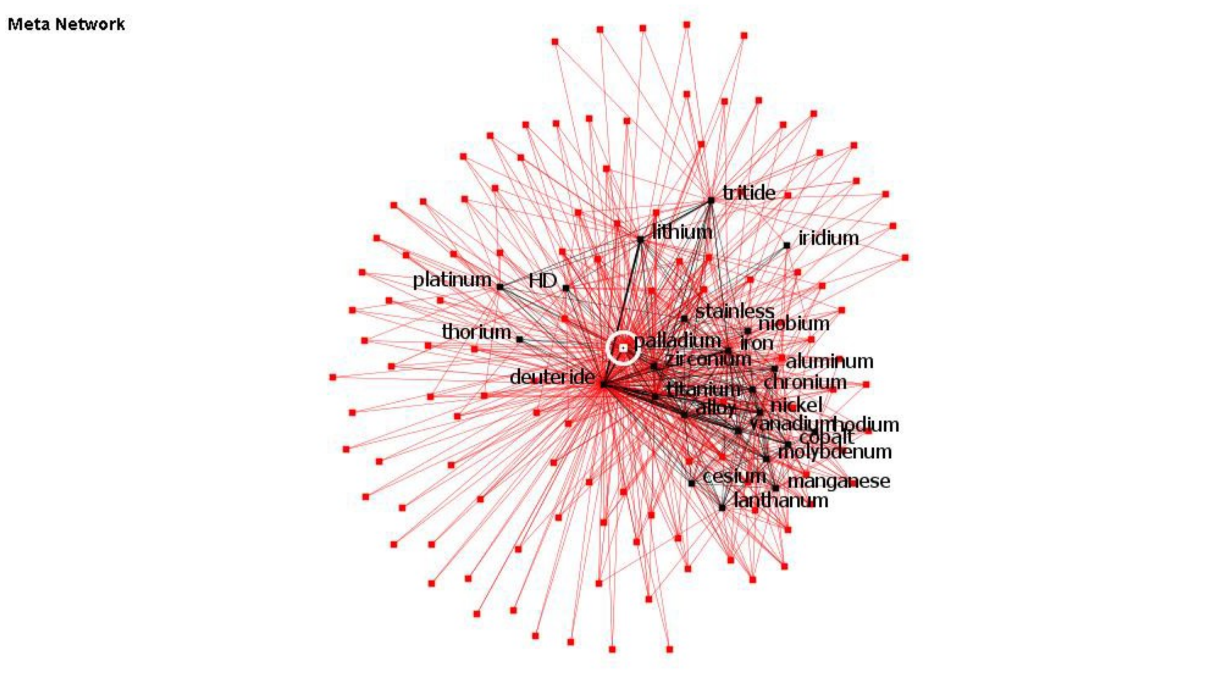


Figure 20: 1st Degree Network of Titanium

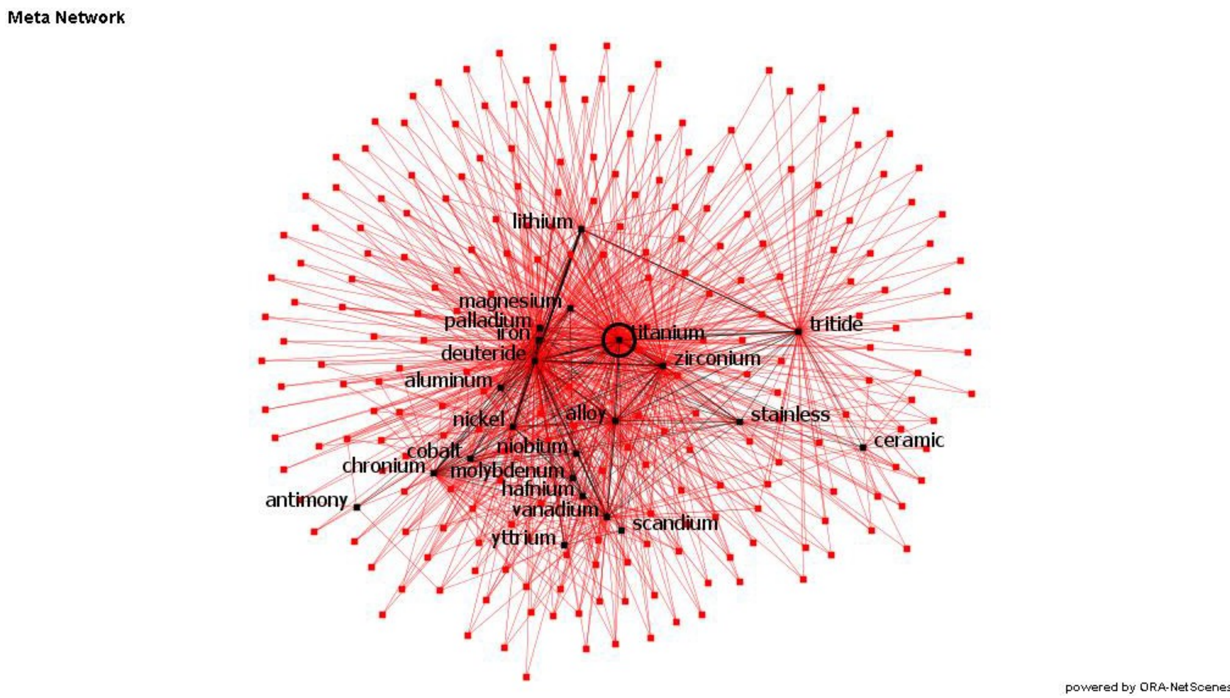


Figure 21: 1st Degree Network of Vanadium

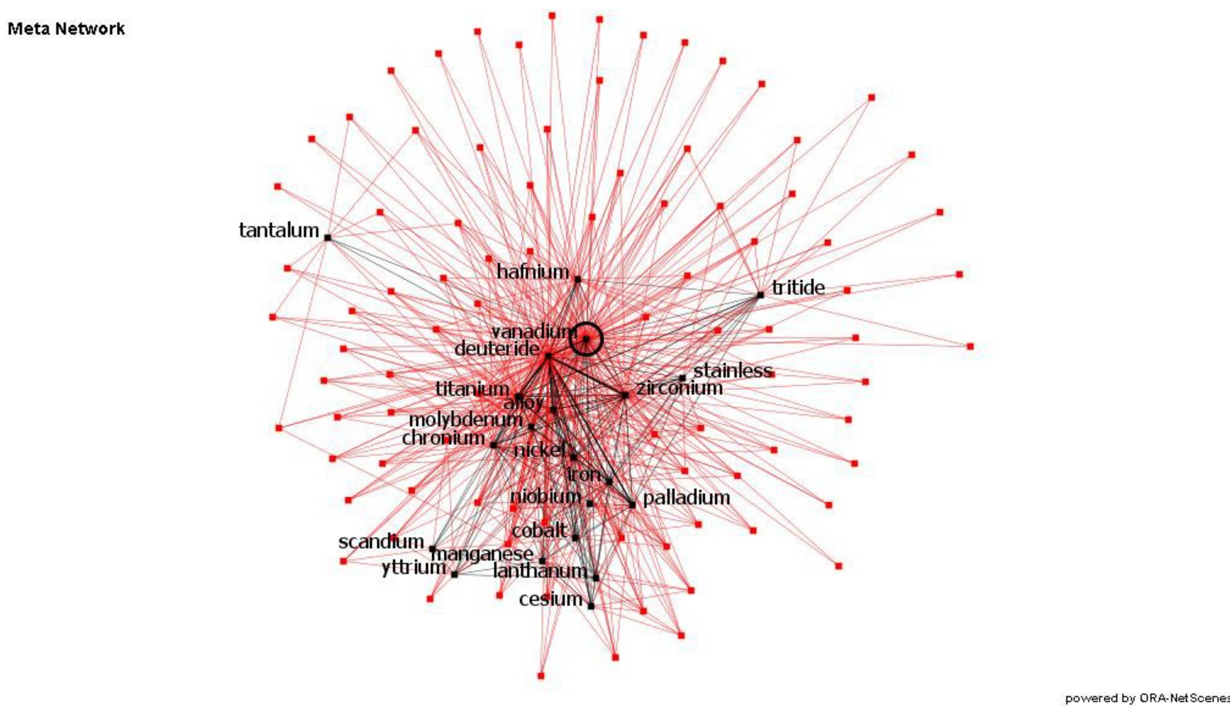


Figure 22: 1st Degree Network of Lithium

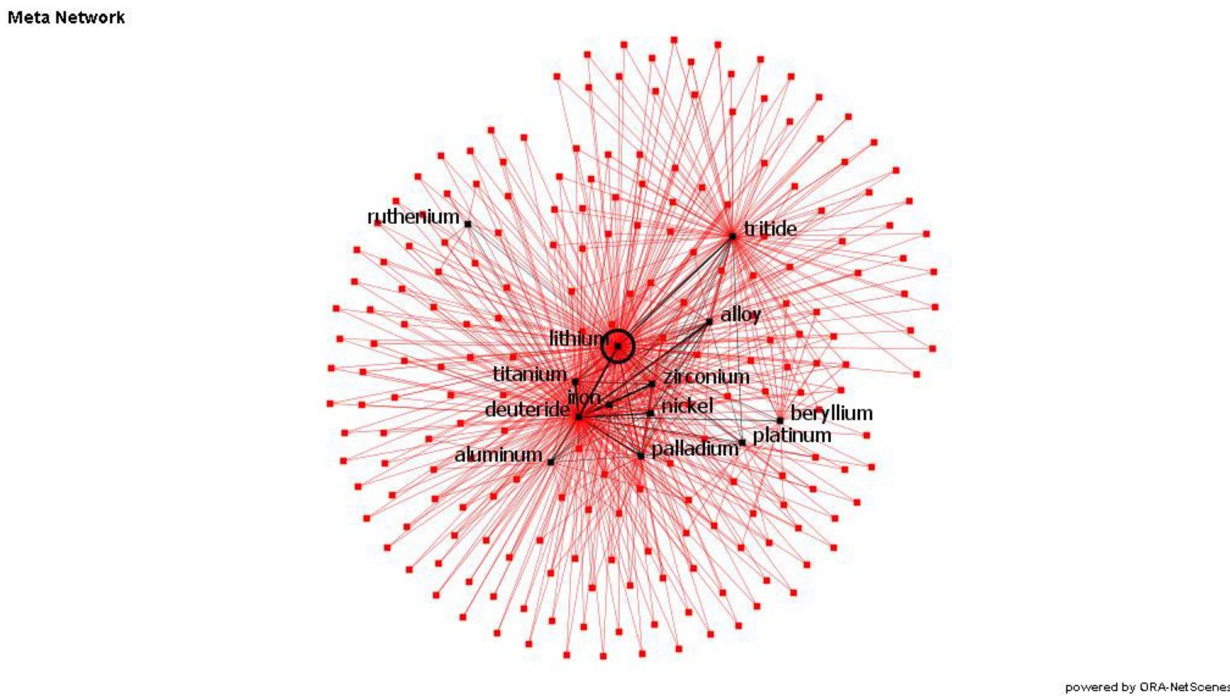


Figure 23: 1st Degree Network of Chromium

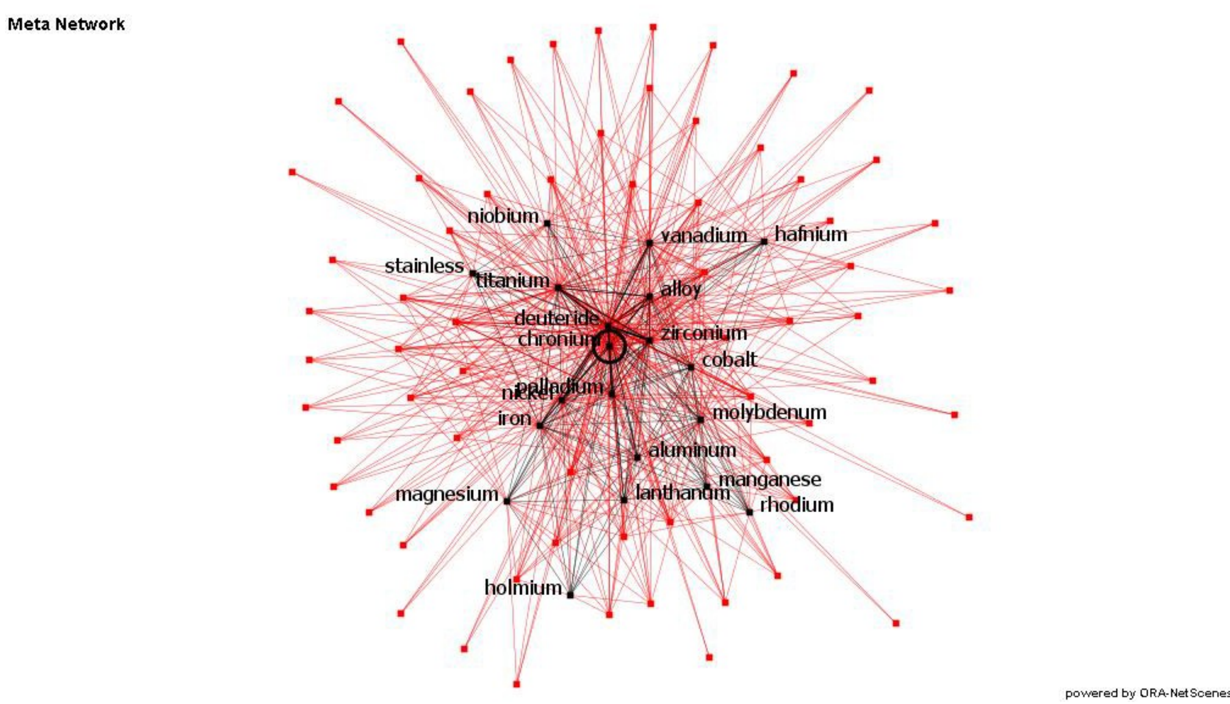


Figure 24: 1st Degree Network of Aluminum

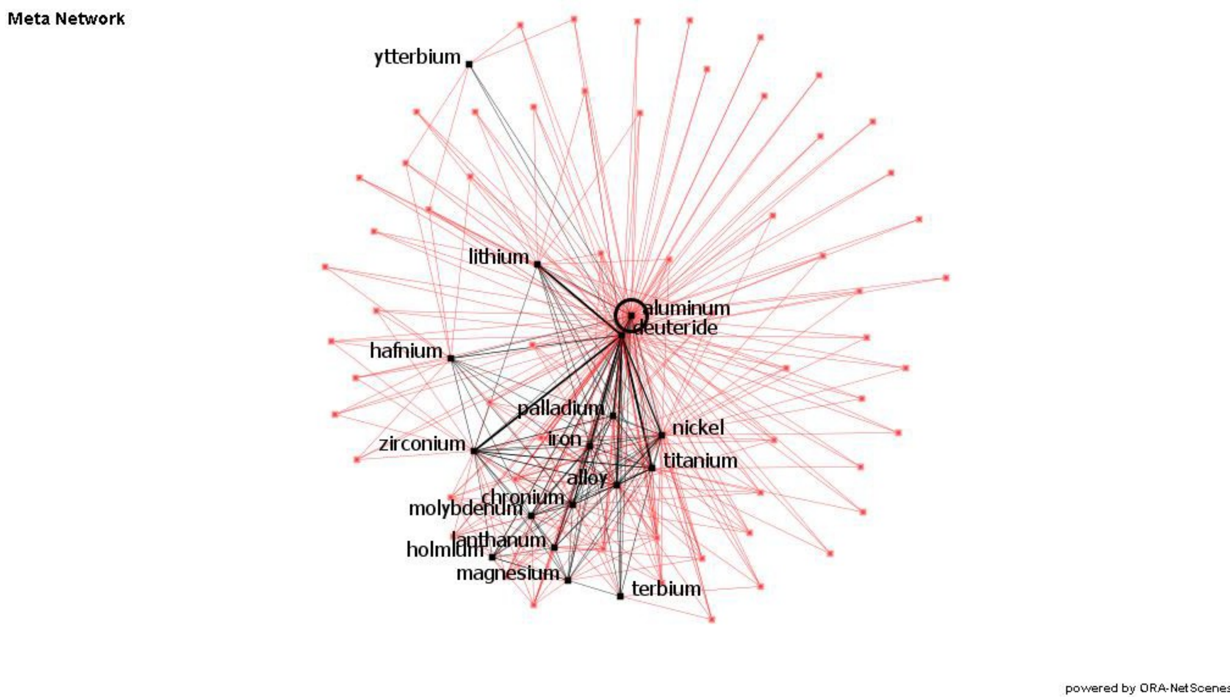
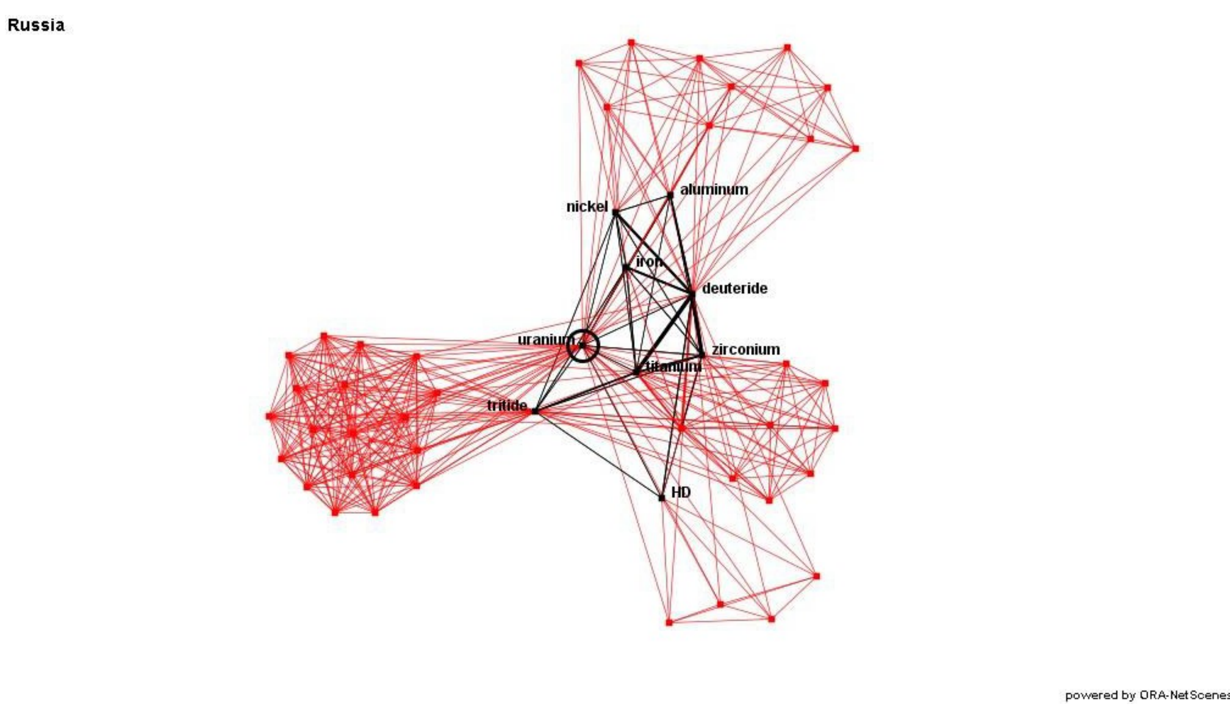


Figure 25: 1st Degree Network of Uranium



The following graphics, Figures 26 through 29, illustrate the link charts for both “deuteride” and “tritide,” including different cluster analysis coloring, to highlight the different materials utilized in each broader research agenda.

Figure 26: 1st Degree Network of Deuteride

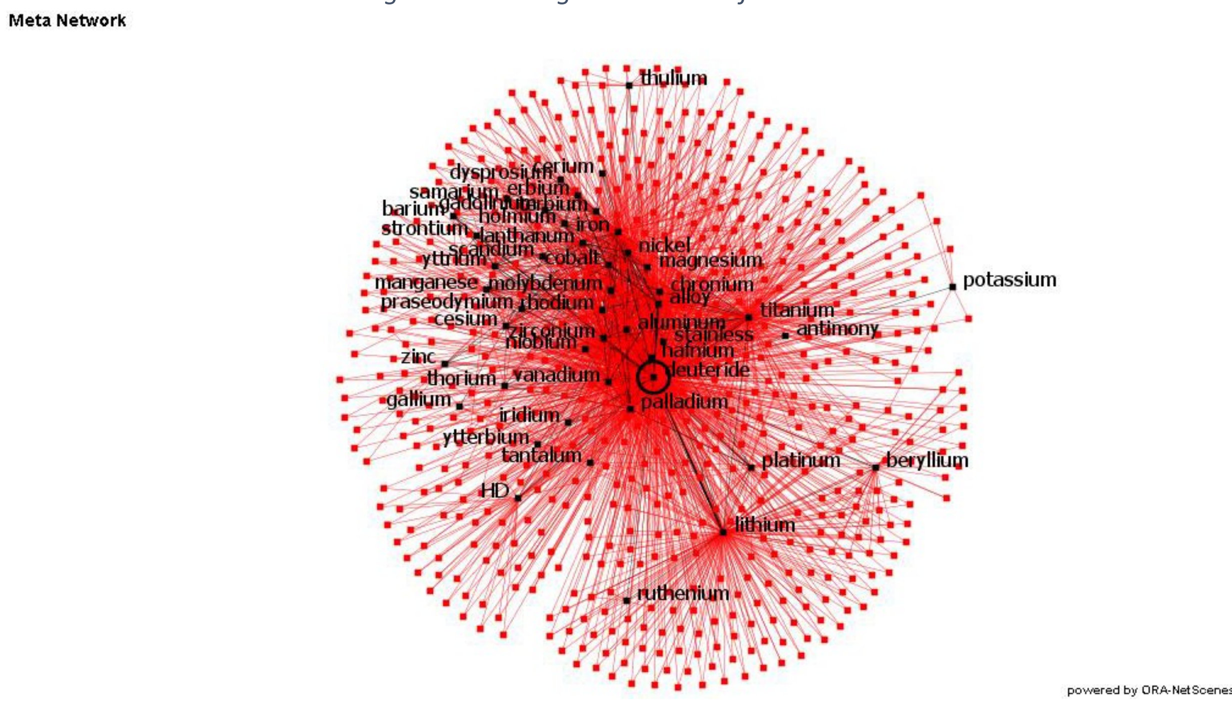


Figure 27: 1st Degree Network of Deuteride – CONCOR Grouping

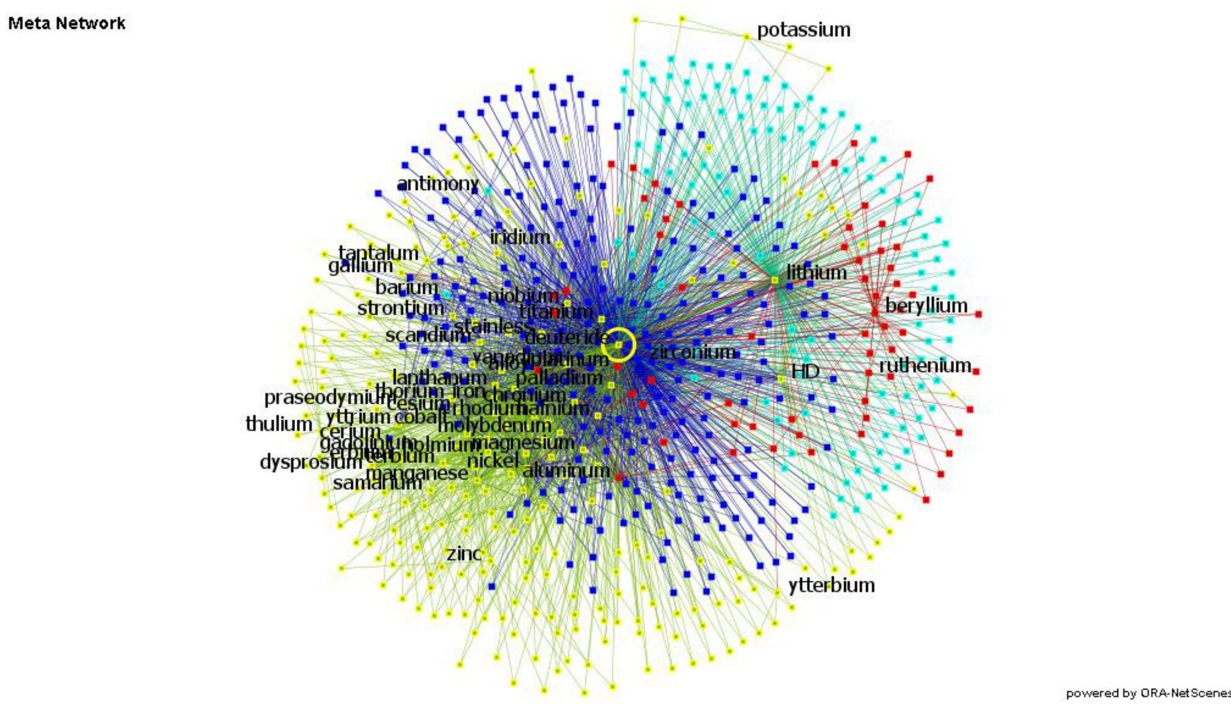


Figure 28: 1st Degree Network of Tritide

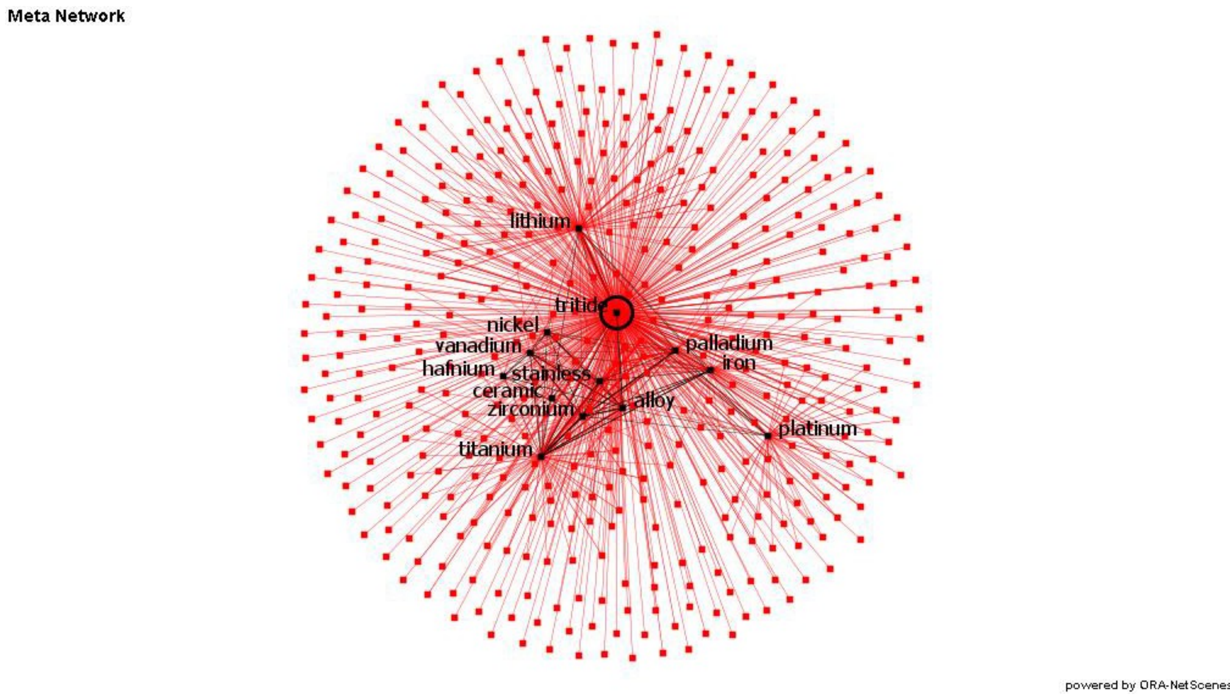
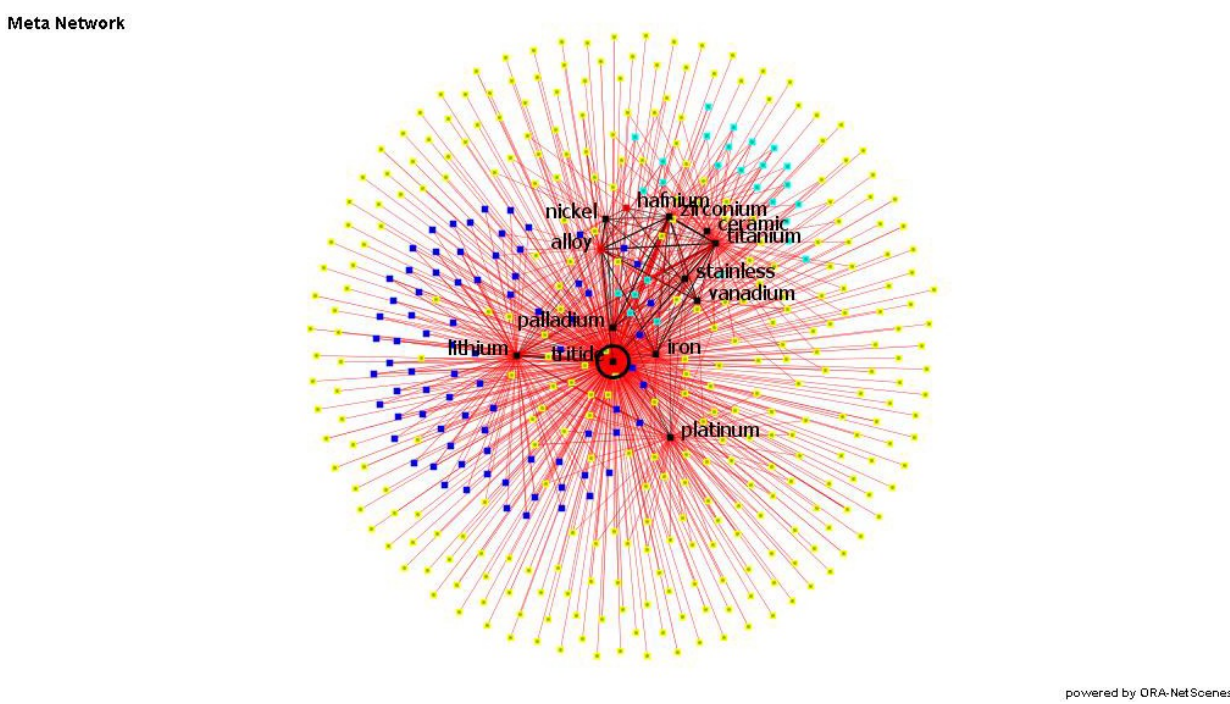


Figure 29: 1st Degree Network of Tritide – CONCOR Grouping



Taking an additional step back from the search parameters, Figures 30 through 34 show the aggregate networks for the entire dataset. This is broken out into graphs for strong ties, those ties with multiple interactions, and all ties, to include weak links of single interaction. Many of the metals included in the network graphs are observed to drop off when the focus is placed on strong ties only. This is the result of the metal being included in the research sparingly or there are very limited research teams engaging the material.

Figure 30: Aggregate Network with Strong Ties Only

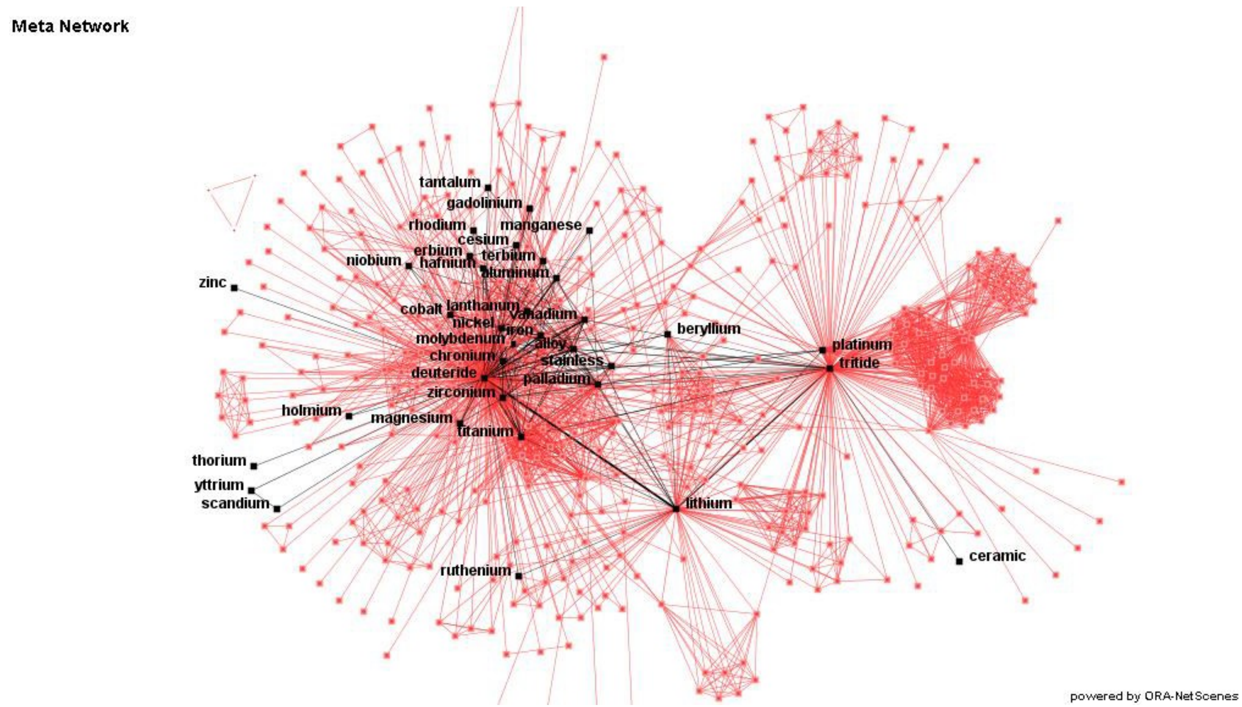


Figure 31: Aggregate Network with Strong Ties Only and CONCOR Grouping

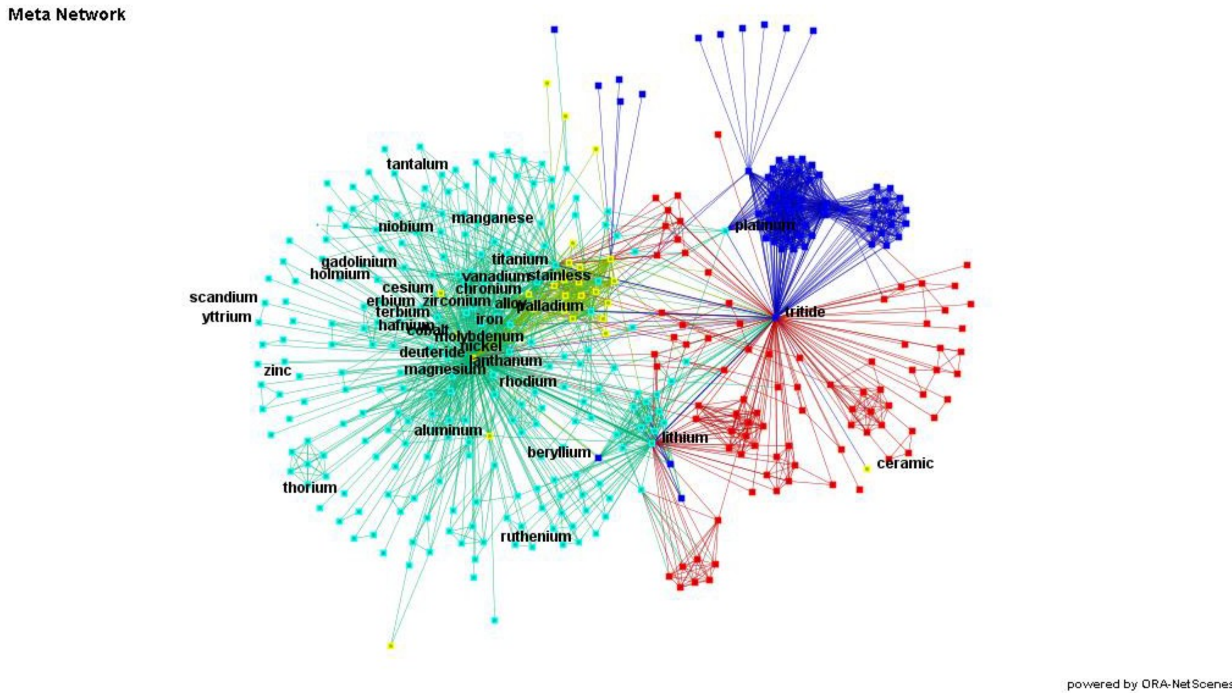


Figure 32: Aggregate Network with Strong Ties Only and Newman Clustering

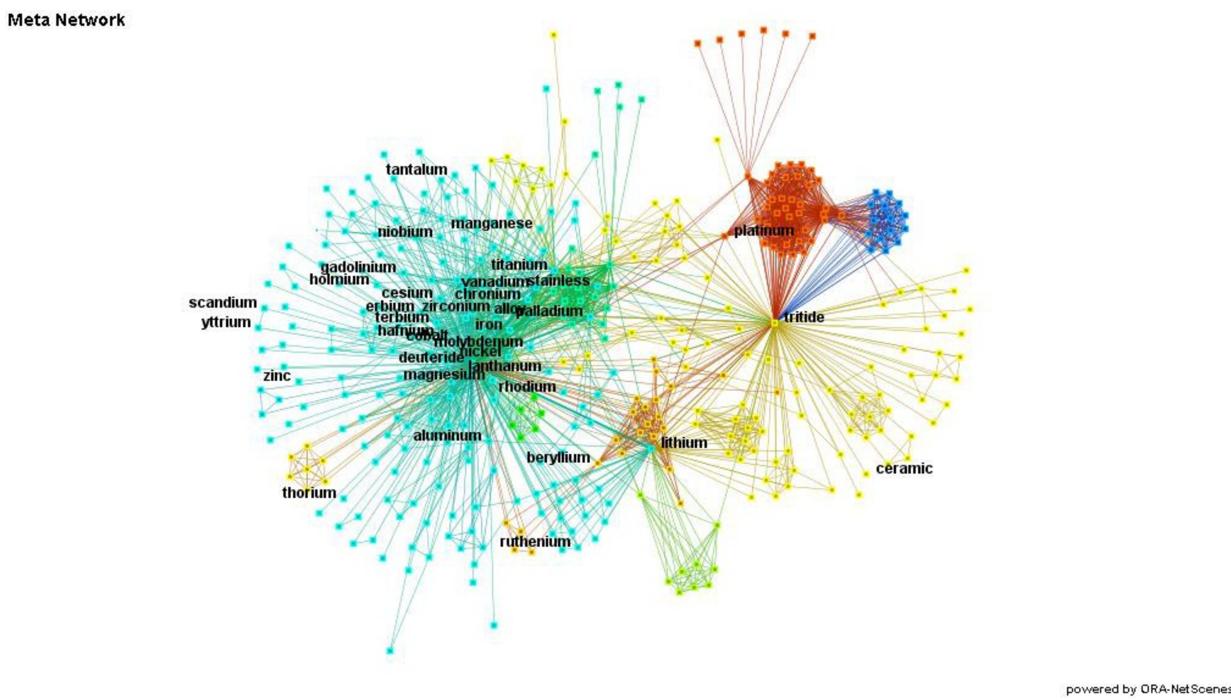


Figure 33: Aggregate Network with all Connections and CONCOR Grouping

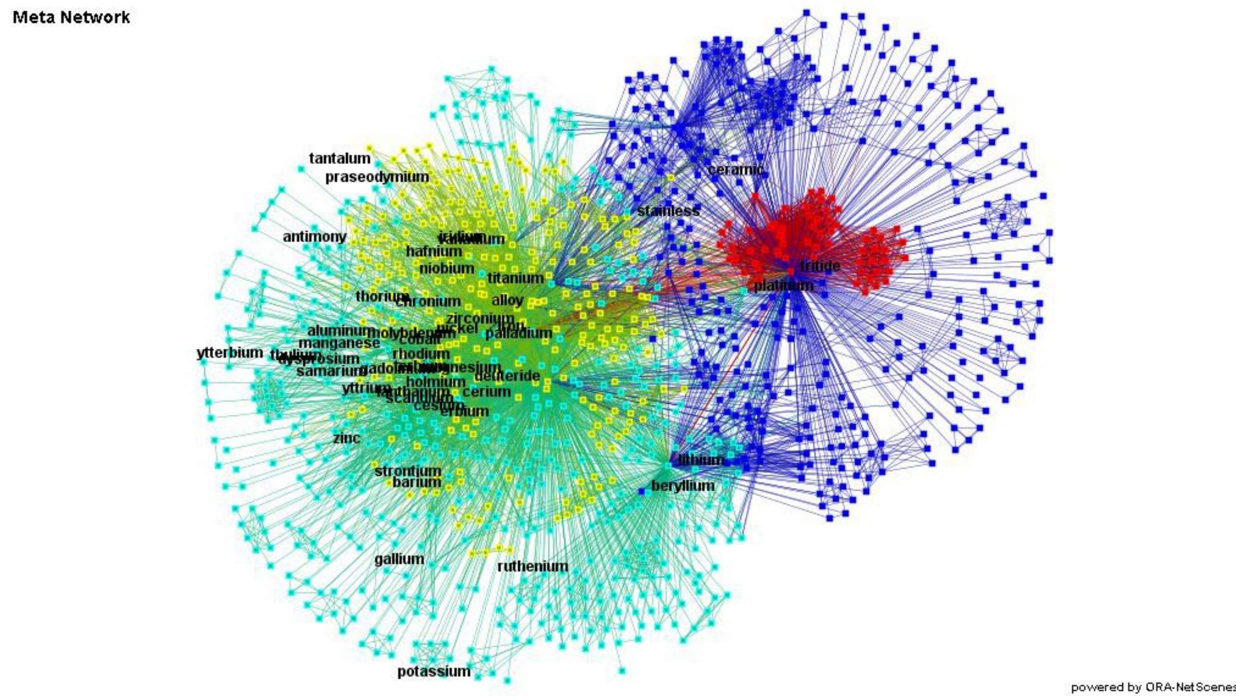
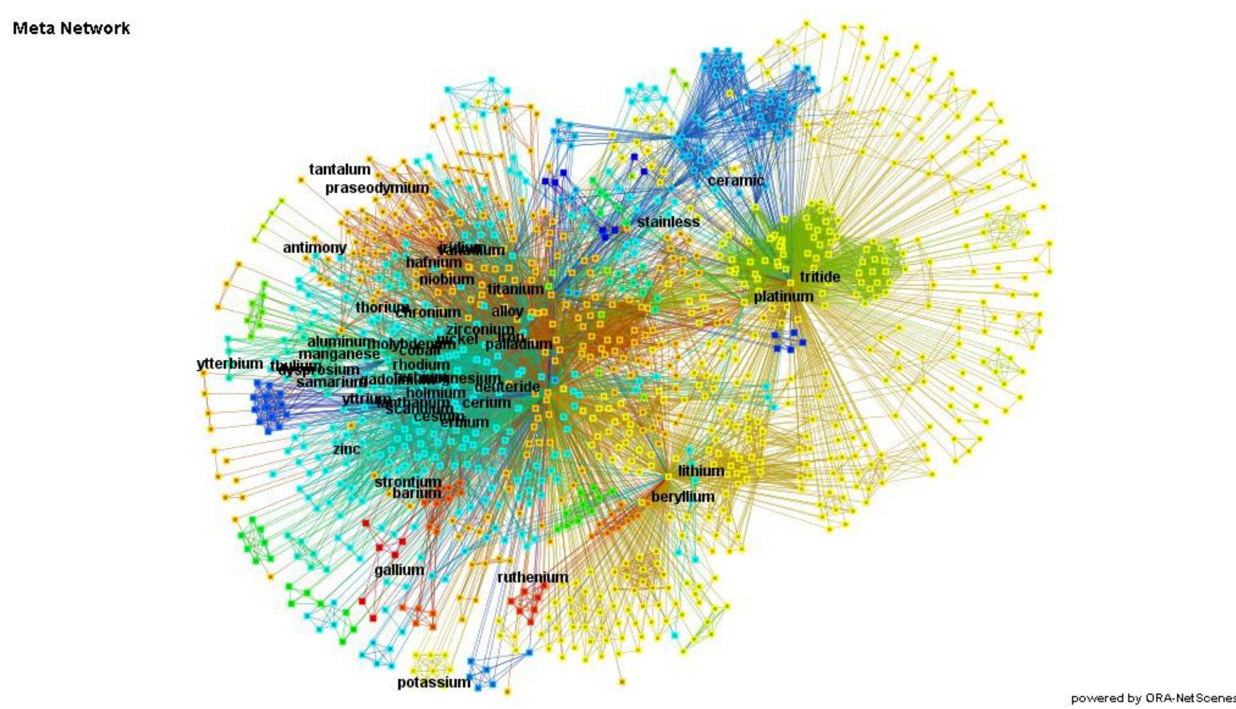


Figure 34: Aggregate Network with all Connections and Newman Clustering



Observations

The following research has attempted to model the different scientific networks engaged in the study of metal hydrides and solid-state hydrogen storage techniques in Russia. While the original objective was to focus on individuals and organizations, the scope of the research was adjusted to focus on the materials being used. Figures 15 through 34 above have attempted to illustrate the interaction of different materials that were present in the research focused on “deuteride” and “tritide.” As the author is not an expert in metal hydrides, no conclusions will be made on noteworthy use of particular materials demonstrated in the network graphics. With that said, from a network perspective, there are a few interesting observations.

First, there is limited significant technical overlap in the materials used in research for “deuteride” and “tritide.” The network graphs and data show that only titanium and lithium have substantial collaborative research networks for both “deuterides” and “tritides.” Given the lack of technical expertise, it was noted as interesting that there was overlap on two descriptive characteristics, but greater usage on the “tritide” side – stainless and ceramic.

Second, the “deuteride” technical community has a significantly greater number of varying metals and materials and more complex network configuration than that of the “tritide” network. This may be a result of the quality of material acquired during the search phase or stemming from the dominant role of a few metals in this research.

Third, the CONCOR clustering was interesting for both the “deuteride” and “tritide” networks, as well as the aggregate networks. Allowing for breakouts of four groups for each network graph, the link chart generally highlights distinct groups. These splits seem to occur logically between “deuteride” and “tritide,” and then within each of these groups. On the “tritide” side, the divide appears between those working with platinum, and those who are not. On the “deuteride” side, the separating classification appears difficult to distinguish given the lack of technical expertise by the author. That said, the split does appear to engage a dense cluster of materials, with peripheral materials forming their own groupings. The Newman clustering visualizations generally align with the CONCOR grouping, but are broken out further into subgroups, allowing for a bit more clarity on the deuteride side.

Finally, it is worth noting that the most dominant metals observed in the research were titanium, zirconium, lithium, nickel, and iron, as well as alloys. That said, it was surprising the variation that was observed in the different metals that were used in the research. From a network statistics level, palladium, chromium, and vanadium were also significant in the meta-network, as demonstrated with large triad count, authority centrality, and effective network reach – indicating both density and interconnectivity. Additionally, in looking at the node-level network statistics for each metal, presented in Table S1, some interesting observations from a network analysis perspective are highlighted. For example, while alloy was one of the more present factors in the network graphs and networks overall, the statistical indicators show that it is critical, this importance is relatively localized to a smaller community in terms of interaction with metals. Conversely, iron and nickel both have significant usage across the network in terms of the meta-network indicators, but limited interaction with the more dominant metals of the network, as shown in the network graphs.

Table S1

Material	Authority Centrality	Capability	Clique Count	Clustering Coefficient	Constraint	Effective Size	Eigenvector Centrality	Hub Centrality	Total Degree Centrality	Triad Count
alloy	0.50	0.70	27	0.44	0.36	149.91	0.43	0.50	0.06	154
aluminum	0.19	0.21	10	0.63	0.44	39.99	0.14	0.19	0.02	85
antimony	0.01	0.01	1	1.00	0.77	1.00	0.01	0.01	0.00	1
barium	0.01	0.02	1	1.00	0.38	3.54	0.01	0.01	0.00	15
beryllium	0.09	0.01	1	1.00	0.88	12.07	0.06	0.09	0.01	1
ceramic	0.01	0.01	1	1.00	0.51	3.26	0.01	0.01	0.00	3
cerium	0.01	0.02	1	1.00	0.50	2.29	0.01	0.01	0.00	6
cesium	0.08	0.10	5	0.64	0.36	23.39	0.06	0.08	0.01	50
chromium	0.23	0.30	15	0.69	0.36	62.18	0.18	0.23	0.03	118
cobalt	0.11	0.15	6	0.74	0.37	27.53	0.08	0.11	0.01	78
deuteride	0.48	0.99	47	0.21	0.15	483.99	0.87	0.48	0.19	217
dysprosium	0.01	0.02	1	1.00	0.45	2.70	0.01	0.01	0.00	10
erbium	0.08	0.06	4	0.76	0.36	22.60	0.06	0.08	0.01	34
gadolinium	0.04	0.06	4	0.71	0.34	12.24	0.03	0.04	0.01	32
gallium	0.01	0.01	1	1.00	0.63	1.44	0.01	0.01	0.00	1
hafnium	0.14	0.06	3	0.89	0.46	28.92	0.10	0.14	0.01	40
HD	0.10	0.02	4	0.80	0.55	15.57	0.07	0.10	0.01	8
holmium	0.03	0.10	5	0.72	0.27	12.32	0.02	0.03	0.01	56
iridium	0.01	0.01	1	1.00	0.63	1.63	0.01	0.01	0.00	3
iron	0.33	0.75	29	0.45	0.33	95.71	0.26	0.33	0.04	170
lanthanum	0.09	0.30	9	0.61	0.30	28.43	0.07	0.09	0.01	104
lithium	0.44	0.08	6	0.62	0.49	95.51	0.34	0.44	0.04	41
magnesium	0.06	0.06	2	0.96	0.36	14.26	0.04	0.06	0.01	43
manganese	0.06	0.12	6	0.82	0.34	15.62	0.05	0.06	0.01	75
molybdenum	0.08	0.21	12	0.76	0.32	24.34	0.06	0.08	0.01	104
nickel	0.35	0.75	26	0.43	0.34	103.61	0.28	0.35	0.04	164
niobium	0.05	0.03	2	0.95	0.43	9.82	0.04	0.05	0.00	20

Table S1 (continued)

palladium	0.39	0.50	23	0.52	0.43	95.61	0.31	0.39	0.04	132
platinum	0.11	0.03	4	0.90	0.47	23.67	0.08	0.11	0.01	19
potassium	0.01	0.01	0	0.00	1.00	1.00	0.01	0.01	0.00	0
praseodymium	0.01	0.01	1	1.00	0.59	1.62	0.01	0.01	0.00	3
rhodium	0.03	0.05	2	0.97	0.35	8.56	0.03	0.03	0.00	35
ruthenium	0.02	0.01	1	1.00	0.86	3.05	0.02	0.02	0.00	1
samarium	0.01	0.02	1	1.00	0.45	2.70	0.01	0.01	0.00	10
scandium	0.03	0.04	3	0.82	0.36	7.28	0.02	0.03	0.00	23
stainless	0.10	0.10	6	0.71	0.34	28.00	0.08	0.10	0.01	55
strontium	0.01	0.02	1	1.00	0.38	3.54	0.01	0.01	0.00	15
tantalum	0.02	0.01	1	1.00	0.73	3.20	0.02	0.02	0.00	1
terbium	0.08	0.08	7	0.61	0.35	23.39	0.06	0.08	0.01	40
thorium	0.02	0.02	2	0.93	0.42	5.16	0.02	0.02	0.00	14
thulium	0.01	0.01	1	1.00	0.67	1.26	0.01	0.01	0.00	1
titanium	0.55	0.45	19	0.49	0.40	148.99	0.49	0.55	0.06	114
tritide	0.15	0.12	9	0.58	0.24	75.86	0.16	0.15	0.03	53
uranium	0.02	0.04	4	0.79	0.33	7.25	0.02	0.02	0.00	22
vanadium	0.37	0.34	16	0.59	0.42	91.18	0.30	0.37	0.04	112
ytterbium	0.01	0.01	1	1.00	0.75	1.34	0.01	0.01	0.00	1
yttrium	0.05	0.12	7	0.54	0.28	14.90	0.03	0.05	0.01	49
zinc	0.02	0.02	1	1.00	0.44	4.36	0.02	0.02	0.00	10
zirconium	0.53	0.70	31	0.44	0.41	146.74	0.46	0.53	0.06	156