Developing Interoperable Ontologies for Research Data Management in the Energy Domain

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Abstract
Currently there is no general shared approach for research data management in the energy system research community, which hinders the reuse of data and software in this domain. The NFDI4Energy consortium is developing several ontologies for use in a research data management platform for energy system researchers. The planned domain ontology for energy system research will form the basis for multiple ontologies with more specialized focus areas; therefore, all specialized ontologies must be designed for interoperability with this domain ontology and with each other. This paper presents an overview of the first stages of the ontology development process, with a focus on the domain ontology. It describes the scope and purpose of this ontology and the methodology for its ongoing development. Requirements for the ontology are summarized, and guidance is provided for future ontology development in the energy domain.

Keywords
ontology, energy, energy systems, research data management, FAIR data, metadata, Semantic Web, NFDI4Energy, NFDI

1. Introduction

Open science ensures the reproducibility of research findings. It also supports better control and organization of data, even if these findings are not reproducible. This guarantees scientific progress [1]. All research fields should therefore move towards open science. In light of the worsening climate crisis, this is especially the case for energy research.

The energy research domain is complex and multi-faceted. It is often too expensive or even impossible to conduct field tests for all experiments. Because of this, energy research heavily

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relies on simulation to test hypotheses. Simulation experiments use a substantial number of digital objects, such as power network topologies and power usage datasets, but only a small number of researchers publish this data according to the FAIR (Findable, Accessible, Interoperable, Reusable) [2] principles. Without adhering to these principles for good data management, digital objects become difficult, if not impossible, to access and reuse.

Addressing this need is our goal as part of the NFDI4Energy consortium, which is one of 26 consortia in the German NFDI (Nationale Forschungsdateninfrastrukur/National Research Data Infrastructure) association [3]. Each NFDI consortium includes researchers from across Germany who are working to improve research data management (RDM) in their particular scientific domain.

In NFDI4Energy, we plan to create an RDM platform that supports the use of FAIR digital objects in the energy research domain. It provides several services for users with varying levels of expertise in energy research [4]. To ensure that the final platform covers the RDM needs of such a diverse user base, the consortium will collect user data through various channels, such as surveys and workshops.

With this platform, which is currently under development, we aim to facilitate data management tasks like adding metadata to digital objects and enhancing their FAIRness. For this, we need more than just general metadata standards such as DataCite[1]. We need specialized standards containing domain knowledge. Therefore, we develop several ontologies simultaneously, covering different aspects of energy systems research.

The main focus of this development is the energy system research domain ontology. It serves two purposes: providing a controlled vocabulary to define domain metadata for existing digital objects and forming the core of the RDM platform's semantic layer. It is the main ontology that all other NFDI4Energy ontologies must be interoperable with. In the rest of this paper, we will call this ontology our domain ontology, as it has the greatest subject area coverage out of all our planned ontologies. The other ontologies are subdomain ontologies. They focus on more specific topics within the energy system research domain. We are developing them to be viable as stand-alone ontologies, but all of them will be interoperable with each other.

This paper describes the initial development of an energy system research domain ontology. After reviewing the existing ontology development methodologies, we selected the NeOn Methodology [5], Semi-Automatic Ontology Development Framework [6] and LOT Methodology [7] as base methods to be reused. All of these ontology development methodologies have similar steps at the beginning: ontology scope definition, ontology requirements definition, existing ontology investigation, and existing ontology selection. Therefore, this work follows the same steps to develop the NFDI4Energy domain ontology.

In Section 2, we outline the planned applications of the ontologies and the proposed ontology scope to cover those applications. We focus on the required interoperability between this domain ontology and the related subdomain ontologies. Section 3 reviews the requirements that this ontology must fulfill, the development challenges stemming from the nature of the energy research domain, and the projected use-cases of the ontology. Sections 4 and 5 delve into the first steps of the ontology development: an investigation into current energy-related ontologies, and the selection of an ontology to extend, respectively. Finally, we examine the

[1]https://datacite.org/

future ontology development plans and conclude the paper in Section 6.

2. Ontology Scope and Applications

We are developing five ontologies with varying scopes and intended use cases for the RDM platform.

- An *energy system research domain ontology* will represent knowledge in the energy systems domain and provide a controlled vocabulary for the other ontologies and for NFDI4Energy's metadata standards. It has the widest scope of all ontologies and will form the basis for the development of the other four that are more specialized.
- A *long-term scenario ontology* will represent long-term energy system scenarios. We are developing it to describe these scenarios with standardized terms, therefore simplifying comparisons between scenarios.
- An *energy simulation software ontology* will represent various software approaches to the modeling and simulation of energy systems. It will form the base for a simulation software registry.
- A *simulation scenario ontology* will represent scenarios of energy system modeling and simulation, and also address hardware-in-the-loop and laboratory testing. With it we can align the scenario definitions of different simulation tools in the consortium and allow their integration into the RDM platform.
- A *socio-political ontology* will represent social and political policy factors which are relevant in energy system models and scenarios.

2.1. Ontology Purpose

NFDI4Energy intends to make each ontology available for use by anyone who needs them for their own research projects or other applications. As the ontologies have different scopes, they are also intended to be used at different stages in the life cycle of a research project. As shown in Figure 1, an energy research project typically goes through five stages. The domain ontology is relevant in all stages as it provides underlying definitions of and relationships between energy domain concepts. These carry through into the four specialized ontologies.

When starting a new project, a researcher first identifies existing work related to their idea, and recruits partners to assist them. Next, the experimental setup is defined, often in the form of energy system scenarios, which can be focusing on the long-term or on the more detailed operational investigation of the energy system. The long-term scenario ontology will help researchers especially in the second phase by standardizing descriptions of scenarios, making it easier to compare one scenario to another.

In the third phase, the research team combines data and models into their desired simulations. Here, two ontologies focusing on distributed simulation, which is usually used for more detailed operational investigation, come into play. The energy simulation software ontology will be used for differentiating simulation software and adding domain-specific metadata to the software registry entries. The simulation scenario ontology will be used to align the different simulation

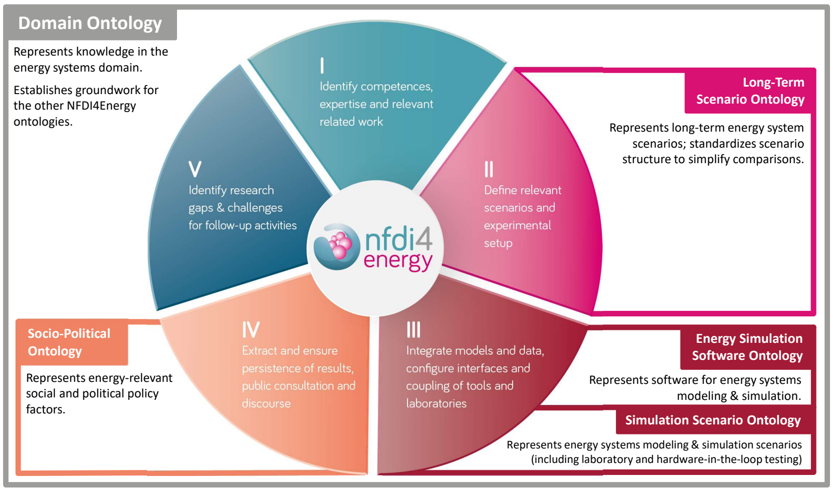

Figure 1: The relationships of the NFDI4Energy ontologies to each other and the five-stage research project life cycle. While the domain ontology encompasses the field as a whole and provides terminology relevant to all stages of an energy systems research project, the other four ontologies will be designed for more specialized use cases at specific project stages. (Figure adapted from [4].)

tools for coupling and will also support the comparison of operational scenarios by supplying additional metadata.

After the research team runs their simulations, the results of their work are disseminated. The socio-political ontology can be of use in this stage, helping to link energy-specific data to the political domain and society as a whole so that non-energy experts can better understand the project's ramifications in relation to non-energy domains. This ontology may also be used earlier when simulations are defined, allowing for socio-political factors to be accounted for in energy system scenarios. Finally, the researchers look for gaps in their work and identify activities for project follow-up, beginning the cycle anew.

NFDI4Energy will support this process by supplying an RDM platform that assists researchers in finding, archiving, and comparing digital objects. We will implement the platform using the developed ontologies as underlying metadata.

2.2. Interoperability

We applied multiple tactics to ensure ontology interoperability and compatibility.

As different teams of experts began developing the ontologies more or less simultaneously, it quickly became apparent that we needed a forum to align the viewpoints of the teams. Therefore, a Metadata & Ontologies Working Group was established shortly after the different teams started working on their respective ontologies. This Working Group aims to improve communication and understanding among the teams, by meeting regularly to discuss overarching issues pertaining to all ontologies being developed and the general development process. This ensures that the ontologies are created with interoperability in mind from the very start of the process and that pitfalls can be identified early and addressed in the working group.

This strategy follows the example of the NFDI association, which supports multiple sections where members of diverse consortia can work together on cross-disciplinary RDM topics [8]. Included is a "(Meta)data, Terminologies, and Provenance" section [9] focused on tasks such as ontology harmonization and mapping. Similarly, other NFDI consortia (e.g., NFDI4Ing [10], NFDI4Earth [11], NFDI4Objects [12], NFDI4Culture [13]) have also formed specialized groups to manage the development of ontologies and other semantic resources among numerous teams.

Further ensuring the interoperability of the ontologies between each other, the working group has determined that all developed ontologies will be built on top of a common top-level ontology. The Basic Formal Ontology (BFO) was selected for this purpose; for further information regarding this choice, refer to section 5. Additionally, the same development process is followed with all the consortium-designed ontologies, ensuring a uniform development and similar design choices, which in turn increases the compatibility between the ontologies.

To address interoperability with ontologies not developed by the consortium, we are considering concepts from ontologies available in the energy domain. The ontologies are analyzed and, if appropriate, concepts from the existing ontologies are used instead of defining them again. Furthermore, we are considering using matching algorithms to bridge between different standard ontologies and the consortium-developed ontologies.

3. Ontology Requirements

The purpose of the domain ontology is to define a fixed set of meanings for its concepts throughout the energy system research domain. As the content base for the other ontologies, its main concern is to portray the domain to the best of its capabilities, while maintaining a certain amount of modularity for interoperability.

As the scope of this ontology is the whole domain of energy system research, the construction of the ontology is not without challenges. The domain is large and complex, containing knowledge from different fields. Thus, without limiting the scope, the development of a holistic ontology for the energy system research domain would not be feasible within a single project, but would be more of a continuous process. Because of these reasons, we have decided to limit the scope of the ontology, making it manageable to construct and use.

To ensure the ontology is constructed within these limits, the team started writing an Ontology Requirements Specification Document (ORSD) early in the development process. This tool was suggested by Suárez-Figueroa et al. [14], and we adapted their template document for our work.

The ORSD contains the requirements for the domain ontology, both at a more abstract level (ontology scope, ontology purpose, etc.) and at a more technical level (implementation language, intended end-users, etc.). It is intended to act as a guide throughout the development process. The team working on the domain ontology filled in the ORSD while consulting the analysis done in other task areas of the consortium. The ORSD is to be consulted when questions arise during the ontology development, to ensure the quality of the ontology created. We present a fragment of the draft ORSD (version 0.5) in Figure 2 to give the reader a sample of its contents.

While the ORSD is still a work-in-progress, the team has already identified and documented some ontology requirements:

- The ontology will be written in the English language and implemented in OWL.
- The ontology will be developed with tools that promote collaborative development.

Ontology Requirements Specification Document	
Ontology Name	NFDI4Energy Domain Ontology
Responsible Team	Task Area 4, Measure 4.1
1	**Purpose**
	This ontology will represent the energy domain and serve as a base for the development of additional ontologies in other TAs and measures, as well as providing a controlled vocabulary for metadata standards.
2	**Scope**
	This ontology will focus on the energy system research domain. Care should be taken that the ontology is not defined too broadly nor too narrowly, as either would make it unusable.
3	**Implementation Language**
	OWL
4	**Intended End-Users**
	• Measure 4.3 team (metadata standards development)

Figure 2: A section of the version 0.5 Ontology Requirements Specification Document (ORSD) for the NFDI4Energy domain ontology. Document template adapted from [14].

- The ontology will reuse concepts from existing ontologies wherever possible.
- The ontology will be applicable to the use cases we define for our RDM platform.
- The ontology will meet requirements identified through input from the expected platform users - the energy industry, the research community, and interested non-experts.

Each of the other developed ontologies will also have its own ORSD, written such that the ontologies will all be developed along similar lines and that the final ontologies will be compatible with each other.

A key component of each ORSD will be a set of competency questions - questions which should be answerable by information encoded according to the terms and relations defined in the ontology. Several development methodologies use this technique as a measure of ontology completeness and accuracy [5, 7, 14]. The terms used in the competency questions also provides developers with insights into vocabulary to consider including in the ontology [14].

4. Existing Ontology Investigation

The Metadata & Ontologies Working Group began the ontology development process of the domain ontology by first examining the current state of the field, collecting a list of 41 existing energy-related ontologies and associated metadata (see Appendix A). The goal of this task was to help determine whether any of these might be suitable starting points for adaptation into the planned ontologies. Since many existing ontologies are open source and include information that falls under the scopes of one or more of the planned ontologies, the consortium intends to reuse these existing resources where possible instead of starting from scratch.

The Working Group then narrowed down the list from 41 entries to 20 entries of the highest interest for the consortium's purposes. We considered criteria such as the scope, licensing, findability, and activity history of each ontology; we gave preference to ontologies more closely matched with NFDI4Energy's needs, with more permissible and open licenses, easily accessible files, and active development teams.

Finally, inspired by the work of the NFDI4Cat consortium [15], the Working Group sorted the remaining 20 ontologies into categories based on their scopes, purposes, and content. This activity allowed team members to take a closer look at each ontology and also further narrowed down the list of potential starting points for the planned specialized ontologies, so that these specialized development teams could focus on just the ontologies that were closest in scope to the use cases of the planned ontologies.

After a discussion-based process, the working group settled on the following categories and definitions for the content of the ontologies:

- *Energy Life Cycle*: Ontologies describing technical aspects of the stages in the life cycle of energy.
  - *Energy Generation*: Ontologies describing the conversion of different energy forms into electric energy.
    - *Renewable Energy Generation*: Ontologies describing conversion methods based on renewable resources (e.g., photovoltaic technologies).
    - *Non-Renewable Energy Generation*: Ontologies describing conversion methods based on non-renewable resources (e.g., coal based electric energy generation).
  - *Energy Storage*: Ontologies describing the storage of electric energy by conversion for later use.
  - *Energy Consumption*: Ontologies describing the consumption of electric energy by conversion.
- *Energy Markets*: Ontologies describing the buying and selling of electric energy.
- *Energy Domain*: Ontologies describing the energy domain as a whole.
- *Smart Grid*: Ontologies describing technologies used in smart grids.
- *Smart Home*: Ontologies describing technologies used in smart homes (e.g., thermostats, appliances, Internet of Things (IoT) devices).
- *Energy Efficiency in Buildings/Construction*: Ontologies describing the efficient use of energy in the construction and use of buildings.
- *Sustainability Factors*: Ontologies describing the sustainable generation and use of energy (e.g., energy efficiency technologies, efficient construction standards, greenhouse gas emission reduction).
- *Society*: Ontologies describing social factors external to the energy domain that have a strong impact on the energy domain (e.g., politics, environment, human behavior).

It quickly became apparent in this categorization process that the content of many ontologies overlapped with different categories and could not be easily limited to a single category. Therefore, we added another layer of categorization to assess the scope of each ontology:

- *Good Match*: This ontology contained only the specified content category at a complete or near-complete level.
- *Broader*: This ontology contained the specified content category at a complete or near-complete level, as well as information relevant to other content categories.
- *Narrower*: This ontology contained some information relevant to the specified content category, but did not offer a complete representation of the content category.

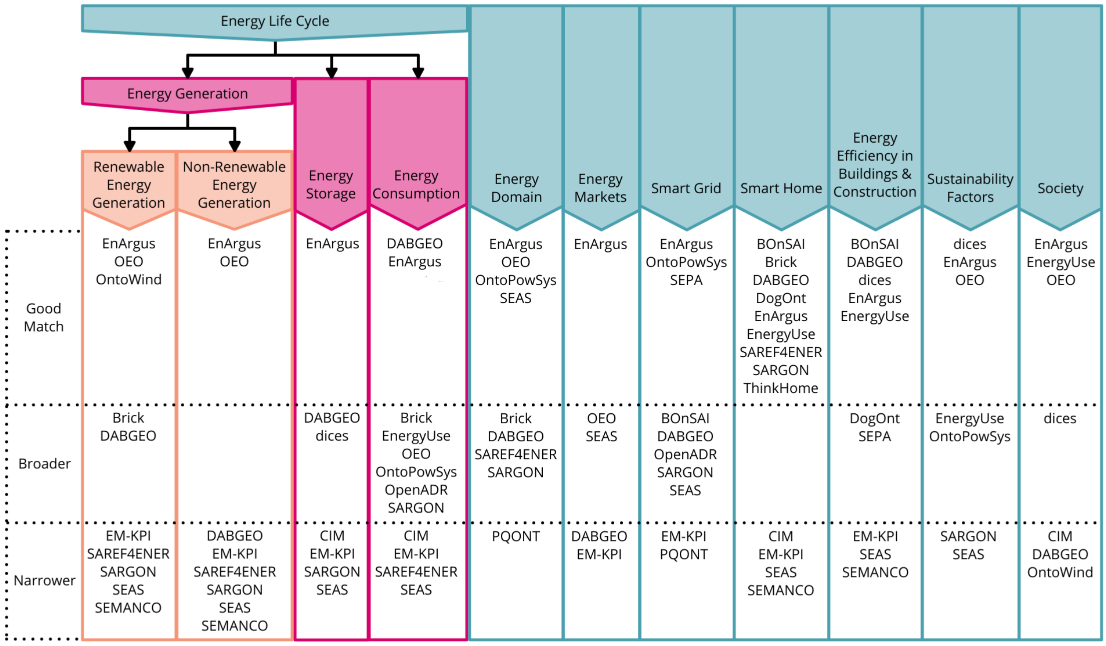

Figure 3: The ontology categorization completed by the Working Group. Content categories are listed across the top, and scope categories are listed along the left side.

We then decided the fit into the scope categories based on the defined scope in the paper or similar document introducing each ontology. The resulting chart (see Figure 3) yielded a precise visualization of the domains of these existing energy-related ontologies of interest, to be used for reference in the further ontology development work.

5. Extension of the Open Energy Ontology

Following the previously described investigation of existing ontologies, the working group opted to proceed in collaboration with the existing Open Energy Ontology (OEO)[2] [16], extending this ontology to fit the needs of the NFDI4Energy platform as the energy system research domain ontology. The OEO was deemed the best option for multiple reasons. It is licensed under CC0-1.0, placing it in the public domain and alleviating any concerns regarding usage permissions. It currently has an active development community with personnel links to NFDI4Energy, which simplifies the process of arranging this collaboration and bringing the NFDI4Energy developers up to speed on the OEO development. Content-wise, this ontology falls into seven of the 11 categories shown in Figure 3, demonstrating that while this ontology still has room for growth, it already covers many topics that are of interest to the consortium. Furthermore, the OEO development is taking place openly on GitHub and the development process is well-defined.

The final key points in the selection of the OEO are features that promote ontology interoperability. For one, the OEO is built according to the BFO, a popular top-level ontology

[2]https://openenergy-platform.org/ontology/

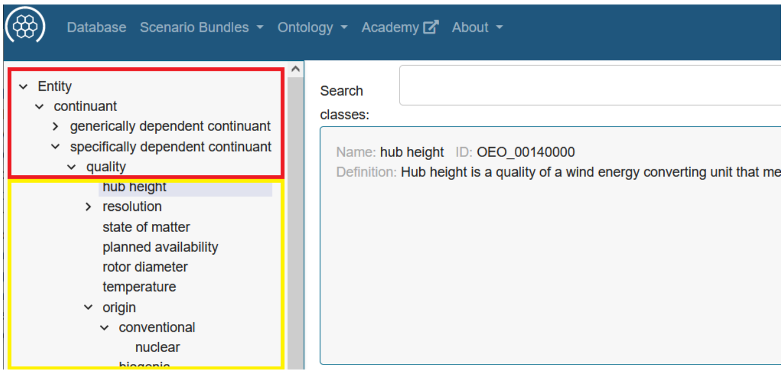

Figure 4: Interaction of OEO classes and BFO classes within the OEO. Terms in the red box come from the BFO, while terms in the yellow box are specific to the OEO. Screenshot from https://openenergyplatform.org/viewer/oeo/ on 16.04.2024; colored boxes for emphasis added by A. Wein.

[17, 18]. Top-level ontologies contain classes and relations between them that are defined at a very abstract level to allow for mapping onto any domain of interest; the BFO in particular is recognized as an ISO standard and is used as a base for over 350 existing ontologies [18]. This gives the ontology development team a wealth of published material from which to learn how to work with the BFO. Use of the BFO as a common ontological base also simplifies the task of mapping terms between separate ontologies, as the structures of two BFO-based ontologies will be quite similar to each other thanks to their generically-defined base concepts. This structure is demonstrated in Figure 4, where domain-specific OEO classes such as "hub height" and "rotor diameter" are established as subclasses of the domain-nonspecific BFO classes "quality," "specifically dependent continuant," "continuant," and finally "entity" at the top of the hierarchy.

Additionally, the OEO allows for flexibility thanks to its modular structure. It is divided into four main modules:

- *oeo-model*: This module contains concepts related to models and modelling of energy systems.
- *oeo-physical*: This module contains concepts of the energy systems sector related to the physical world.
- *oeo-sector*: This module contains concepts regarding sectors and sector division.
- *oeo-social*: This module contains concepts about the social aspects of the energy sector.

An additional *oeo-shared* module contains concepts that are relevant in each of the four main modules, to avoid unnecessary duplication. General class axioms can be found in the supplementary *oeo-physical-axioms* module.

This modularity makes it possible for users to download and use only a small subsection (module) of the ontology if needed. As NFDI4Energy plans to develop multiple ontologies that will be based on the domain ontology and must be interoperable with it, this modular structure yields the possibility of planning our additional ontologies as separate modules of the domain ontology. Through this framework, the domain ontology could either be used as a whole or in smaller parts, with each module having well-defined links to the other modules and to the entire overarching domain ontology.

6. Conclusion

We have outlined the foundational steps taken towards the development of an energy system research domain ontology for the NFDI4Energy RDM platform, from scope and requirements definition to an examination of the currently available ontologies in this field.

The further development of the OEO will be a collaboration between this ontology's current developers and the NFDI4Energy ontology development teams. Our Metadata & Ontologies Working Group will be involved in this process to ensure that each specialized module is fully interoperable with the domain ontology, and that the specifications in each ORSD are met.

Prior to the final releases of the ORSDs, we will define appropriate competency questions for each ontology. Formulating these questions requires a thorough understanding of the use cases for each ontology, ideally with input from the domain experts who will be the end users of the platform. Therefore, the ontology development teams are currently working with the consortium's outreach-focused Task Areas, getting feedback from user groups (energy researchers, the energy industry, societal and political stakeholders) regarding their RDM needs and their expectations for the platform. Each ORSD will include a section with competency questions and a section with potential ontology terms extracted from the questions [14].

With this groundwork laid, we are well-positioned to move forward with the development of the described set of interoperable ontologies to support energy system research with the NFDI4Energy RDM platform.

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A. Ontology List

Table 1
Ontologies listed in alphabetical order. **Bold font** indicates inclusion in the categorization described in Section 4. The version is given for ontologies included in the categorization.

	Abbreviation	Full Name	Version
1		∀Platform ontology	-
2	BFO	Basic Formal Ontology	-
3	**BOnSAI**	**Smart Building Ontology for Ambient Intelligence**	v0.2
4		**Brick**	v1.3
5		Building Energy Ontology	-
6	**CIM**	**Common Information Model**	Multiple.*
7	**DABGEO**	**Domain Analysis Based Global Energy Ontology**	v1.0
8		DECENT Ontology	-
9	DEHEMS	Digital Environment Home Energy Management System Ontology	-
10	**dices**	**Digital Construction Energy**	v0.5
11	DIMMER	District Information Modeling and Management for Energy Reduction	-
12	DNAS	Drivers-Needs-Actions-Systems Ontology	-
13	**DogOnt**	**Domotic OSGi Gateway Ontology**	v1.0
14	ee-district	Energy Efficient District Ontology	-
15		Electricity Markets Ontology	-
16	**EM-KPI**	**Energy Management - Key Performance Indicator Ontology**	v1.1
17		**EnArgus**	v1.0
18		Energy-saving Ontology	-
19		**EnergyUse**	v1.0
20		Facility Ontology	-
21	GAZ	Gazetteer	-
22		Generic Ontology of Energy Consumption in Households	-
23		Integrated heat and electric energy ontology	-
24	LCC	Languages, Countries, and Codes	-
25	NewOSEIM	New Ontological Solution for Energy Intelligent Management	-
26	**OEO**	**Open Energy Ontology**	v2.2.0
27	OEMA	Ontology for Energy Management Applications	-
28	OntoMG	Microgrid Ontology	-
29		**OntoPowSys**	Not found.
30	Onto-SB	Smart Building Ontology	-
31		**Ontowind**	v1.0
32	**OpenADR**	**Open Automated Demand Response Ontology**	v0.2.2
33	**PQONT**	**Power Quality Ontology**	v1.0
34	ProSGv3	Prosumer Oriented Smart Grid Ontology	-
35	**SAREF4ENER**	**Smart Applications REFerence Ontology for the Energy Domain**	v1.1.2
36	**SARGON**	**SmArt eneRGy dOmain oNtology**	v1.0
37	**SEAS**	**Smart Energy Aware Systems Ontology**	v1.1
38	**SEMANCO**	**Semantic Tools for Carbon Reduction in Urban Planning Ontology**	Not found.
39	**SEPA**	**Smart Electric Power Alliance Ontology**	v0.1
40		Solar Soft Cost Ontology	-
41		**ThinkHome Ontology**	Multiple.**

* The CIM ontology is divided into 3 standards. Applicable to this paper are IEC61970 CIM16 v33a, IEC61968 CIM12 v08, and IEC62325 CIM03 v01a.

** The ThinkHome ontology is divided into 5 ontologies with independent versioning. Applicable to this paper are v1.12 (Building Ontology), v1.03 (Energy and Resource Ontology), v1.14 (Process Ontology), v1.01 (Actor and Preference Ontology), and v1.03 (Weather Ontology).