IRO Viewer (Data Journal)

Preservation, Context and Linking

Brian Matthews and Antony Wilson

STFC

ICAT Meeting

Dublin, 25

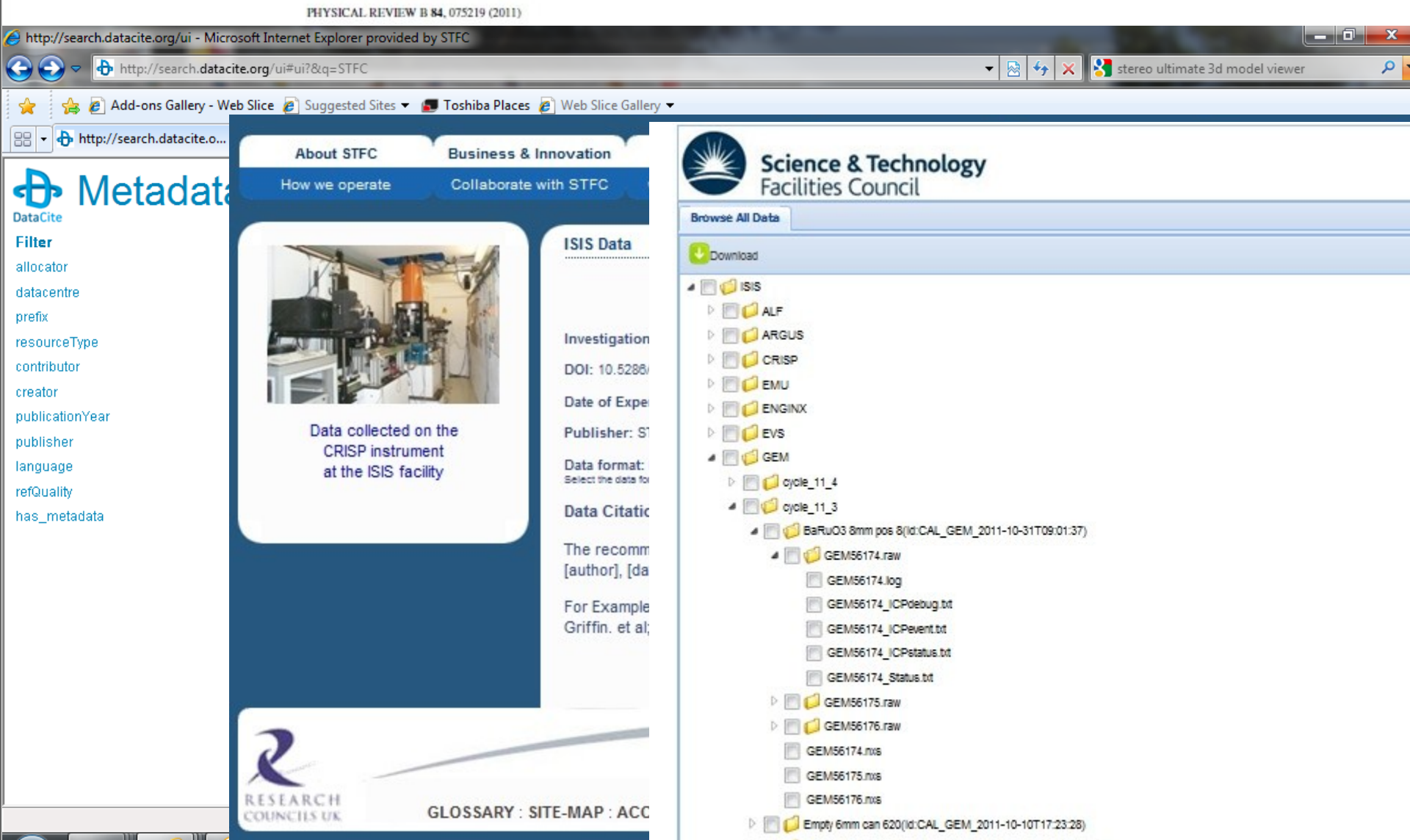
Overview

- Facility data and research objects
- Components
- Demo?
- Preservation
- Summary

This work was partially supported by the SCAPE Project.
The SCAPE project is co-funded by the European Union under FP7 ICT-2009.4.1 (Grant Agreement number 270137).

Facility Data and Research Objects

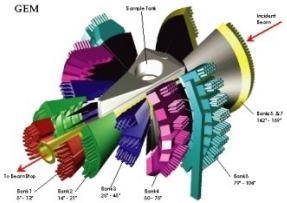
DOI Data Access Process

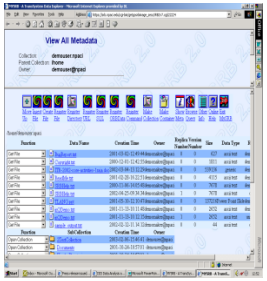


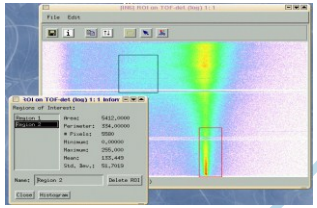
Is this enough?

- What we have so far is good for:
  - us to manage data
  - users to access their own data
  - citation of raw data
- But
  - Publication and exchange of Investigations
    - Traceability and Validation?
    - Reuse of the data?
  - Preservation of Investigations
- Need to make context more explicit
  - Focussing on the dataset is the wrong subject of discourse

Facilities Data Lifecycle







Proposal

Scientist submits application for beamtime

Approval

Facility committee approves application

Scheduling

Facility registers, trains, and schedules scientist's visit

Experiment/ Investigation

Scientists visits facility, run's experiment

Data storage

Raw data filtered, and stored

Data analysis

Tools for processing made available

Record Publication

Subsequent publication registered with facility

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Publishing Investigations

- So what we want is a record of EXPERIMENTS not data.

- Thus want the record of the context
  - The experimental intention and actors
  - The instruments and configurations used
  - The sample
  - The environmental parameters and context
  - The Raw Data
- Thus we want to publish a record of the whole *INVESTIGATION*
  - Can get most of this this from what we have

- The Investigation becomes a “first class” research object
  - Published
  - Identified and treated as a single entity
  - Cited and credited
  - Record of the output of the *facility*

- Analogous to a Journal Article
  - Investigation as the unit of discourse for scientific facilities.

- But also as an access point for validation and reuse
  - Because we have a record of what actually happened.

Our DataCite entries are in fact Investigations

(red is for “data” notion, and green is for “investigation”)

Data collected on the GEM instrument at the ISIS facility

ISIS Data

RB920025.

Investigation title: Crystal and magnetic structures of EuWO1+xN2-x.

Creator: *Kusmartseva,A*
Creator: *Rodgers,J A*
Creator: *Attfield,J P*

DOI: 10.5286/ISIS.E.24071239

Date of Experiment: Tue Aug 04 14:38:23 BST 2009

Publisher: STFC ISIS Facility

Data format: RAW/Nexus
Select the data format above to find out more about it.

DOWNLOAD
download the dataset

Data Citation

The recommended format for citing this dataset in a research publication is as:
[author], [date], [title], [publisher], [doi]

For Example:
Kusmartseva,A. et al; (2009): 920025, STFC ISIS Facility, doi:10.5286/ISIS.E.24071239

Abstract

Eu2+ d0- transition metal perovskites are of interest as potential multiferroics when undoped, or as CMR materials. EuWO1+xN2-x is a new magnetoresistive material and exists over a broad range of x = -0.2 to 0.5. It has a ferromagnetic ordering transition at TC = 12 K. Neutron diffraction is needed to determine the I112/m monoclinic superstructure evidenced by TEM that arises from O/N ordering and octahedral tilting, and the magnetic order. This may include a coexistence of antiferromagnetic/ ferromagnetic orders (as found in a previous GEM study of the analogueEuNbO2N). 2 days on GEM are needed to study 2 samples with different x values (one stoichiometric x =0, the other highly doped x = 0.5) because of high absorption by Eu.

Research Objects

- Represent the “investigation” as a Research Object
  - Research Objects (ROs) are semantically rich aggregations of resources that bring together data, methods and people in scientific investigations. Their goal is to create a class of artefacts that can encapsulate our digital knowledge and provide a mechanism for sharing and discovering assets of reusable research and scientific knowledge
    - www.researchobject.org and elsewhere

- Use RDF, Semantic Web and Linked Data Technologies to support this
  - And we can experiment with these tools for our data

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Building an Investigation Research Object

:investigator

Investigation #n
DOI:STFC.xxx.n

:dataset

:application

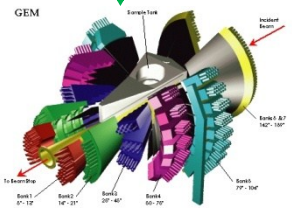
:relatedDataset

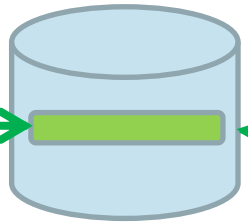
:publication

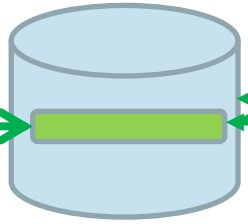
:publication

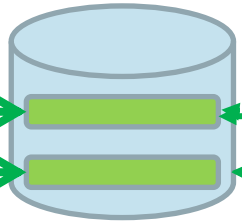
:instrument

:sample





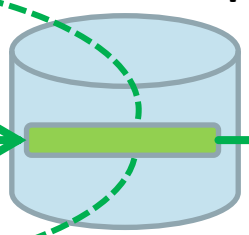


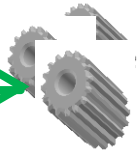


:inputDataset

:outputDataset

Software Repository





Software Package 1

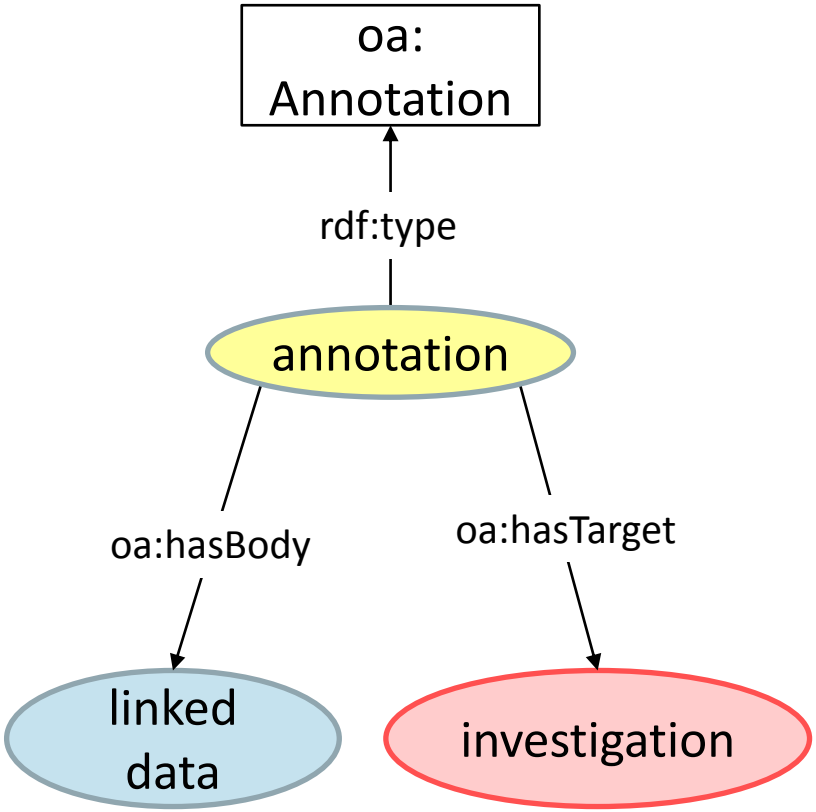
cito:cites

cito:cites

SCAPE

Annotations

- Annotations used to construct a Research Object
  - http://www.w3.org/community/openannotation/
  - More on this later



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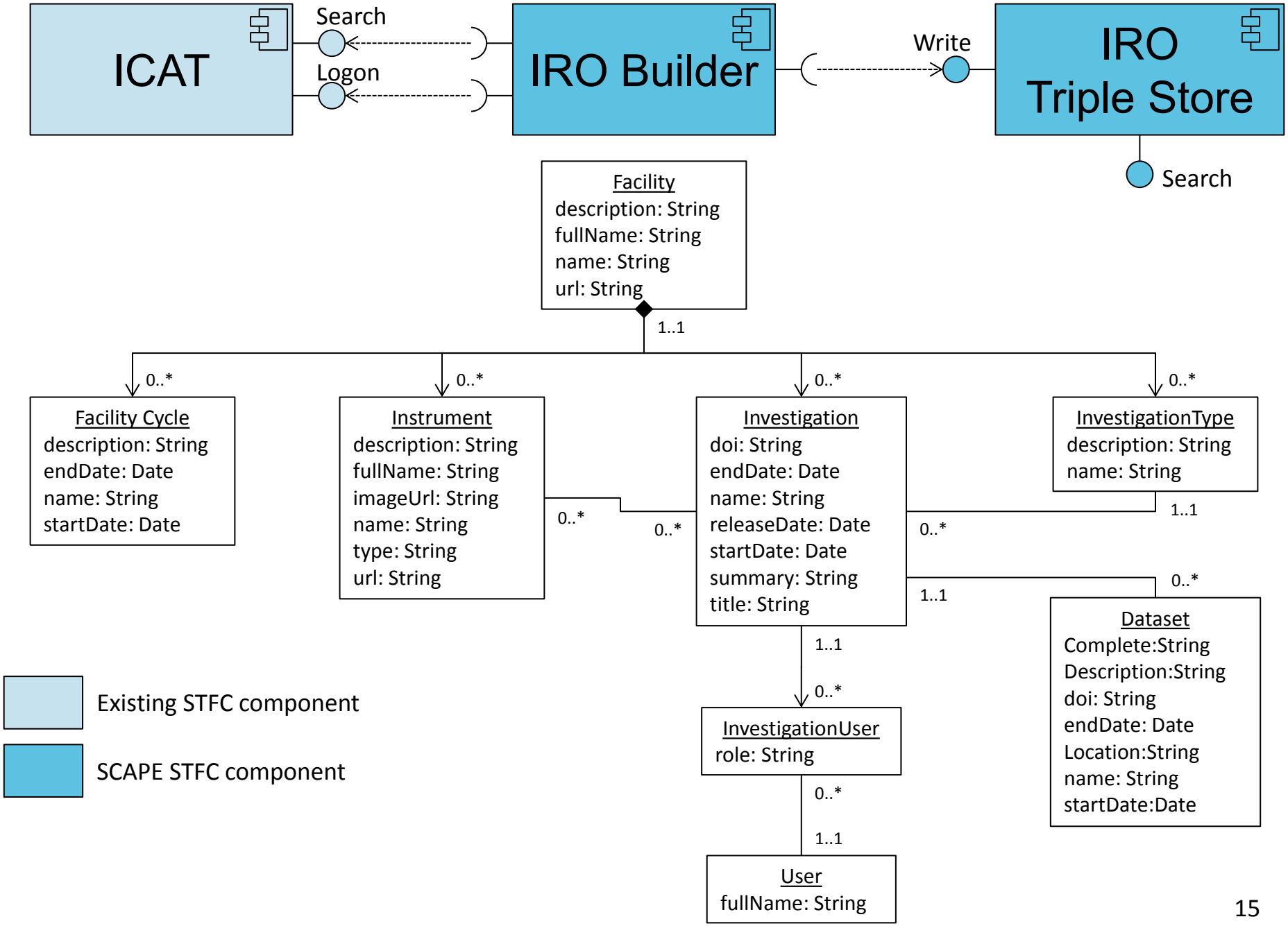
Components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Logon
IRO Builder
Write
IRO Triple Store
Search
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name: String
url: String
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0..*
0..*
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fullName: String
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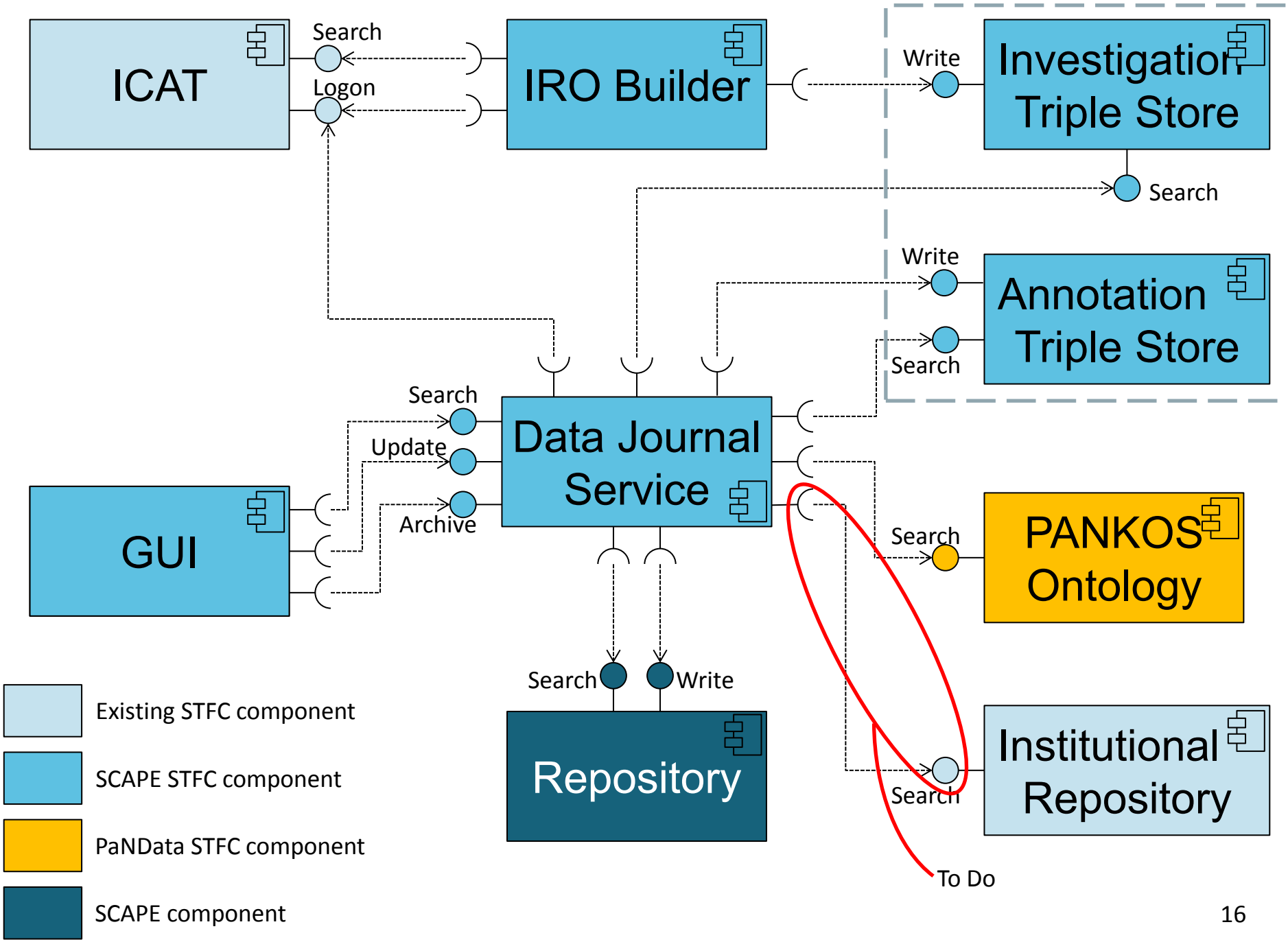
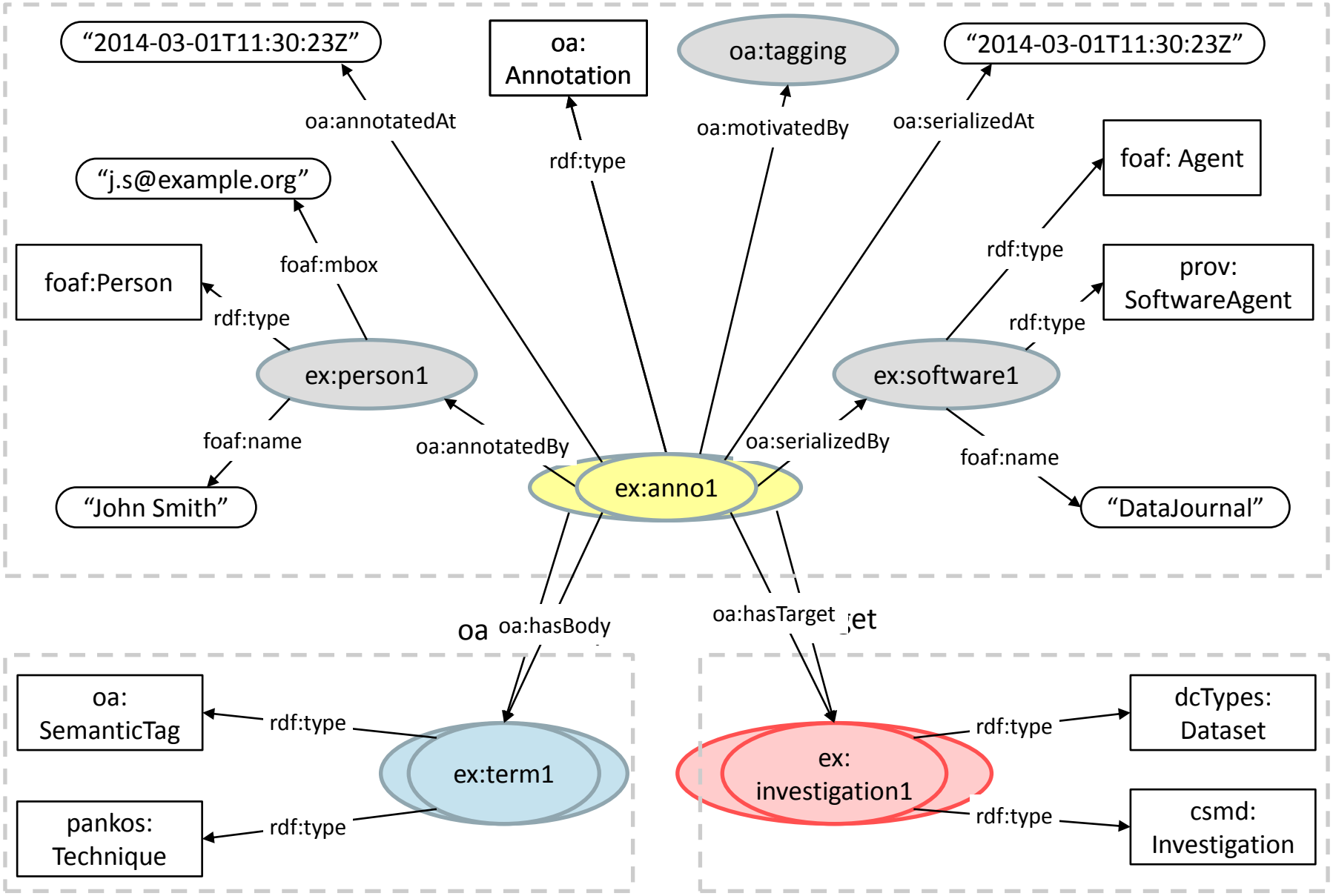
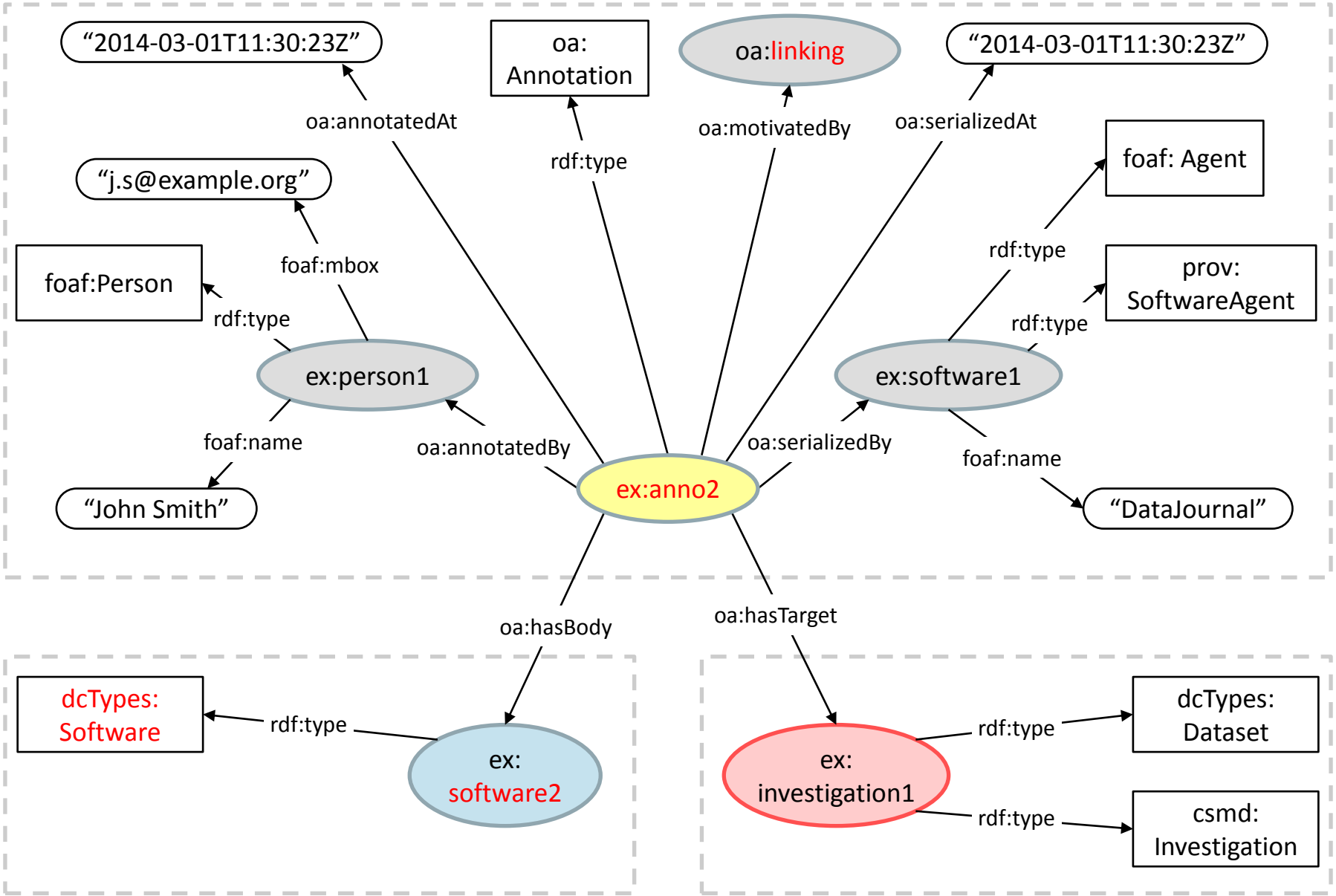
1..1
User
fullName: String
Existing STFC component
SCAPE STFC component


ICAT
Search
Logon
IRO Builder
Write
Investigation Triple Store
Search
Write
Annotation Triple Store
Search
Search
Update
Archive
Data Journal Service
GUI
Search
PANKOS Ontology
Search
Write
Repository
Search
Institutional Repository
To Do
Existing STFC component
SCAPE STFC component
PaNData STFC component
SCAPE component

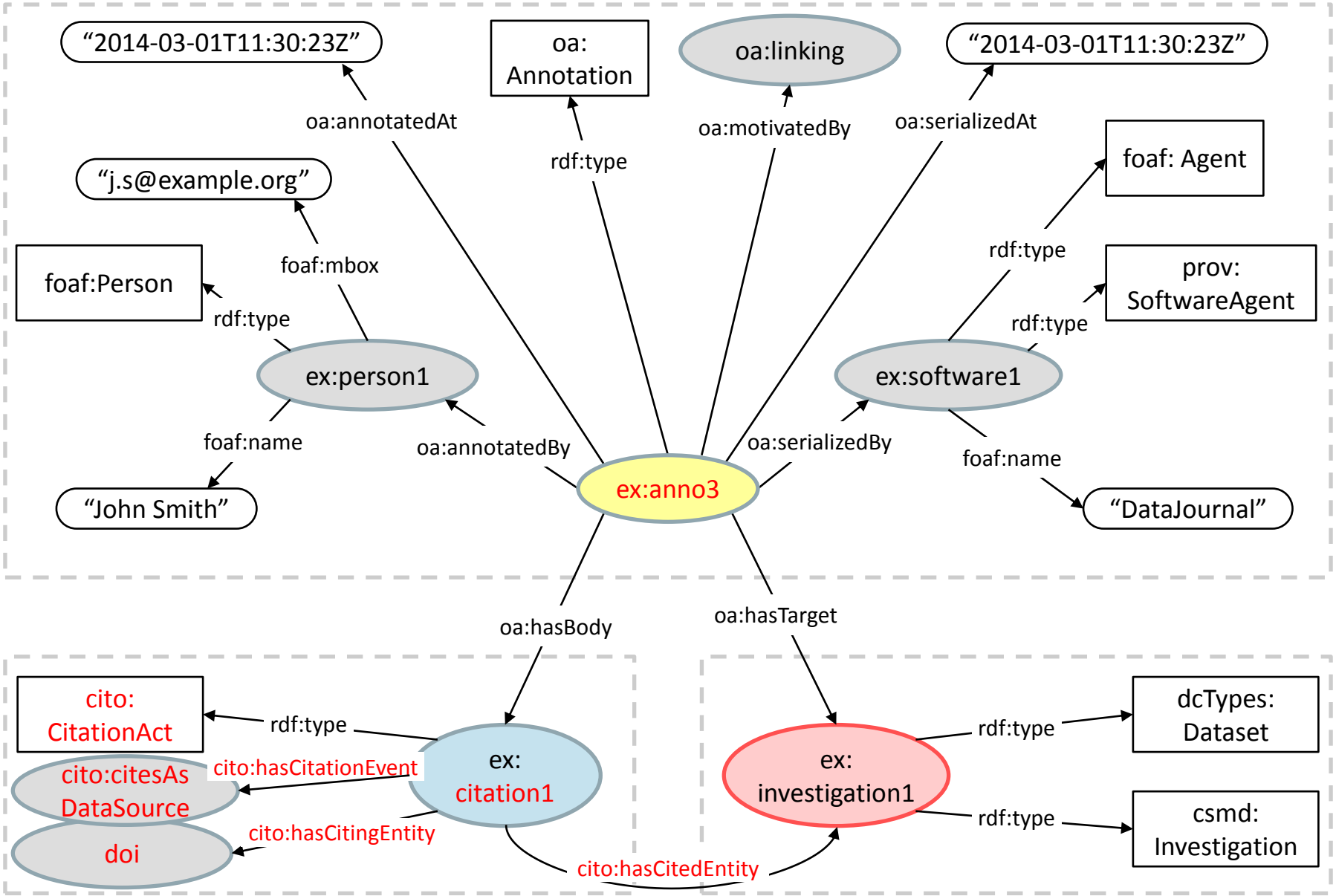
Annotation - Semantic Tagging



Annotation – Linking Software



Annotation – Citations



Demo

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ISIS Data Journal

The archive for ISIS research data

ISIS

Cycles | Investigation | Edit | Archived Versions

This is the main index for the ISIS Data Journal.

There is an entry in the journal for every investigation carried out at ISIS that has a DOI or is no longer in the embargo period. The investigations are grouped into cycles, where a cycle is a period of time during which ISIS was running. The references for the investigation are in the form [Author], [Date], [Title/RB Number], [Publisher], [DOI], where RB Number is a unique number allocated to the investigation. The investigations are sorted by start date. Long running investigations may appear in more than one cycle.

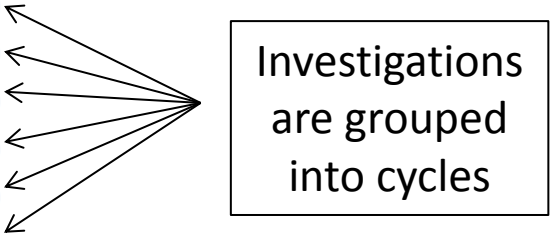
Filters

▶ **Investigation Type**

▶ **Instrument**

Apply

- cycle_13_4 (11/11/2013 - 31/01/2013)
- cycle_13_3 (01/09/2013 - 10/11/2013)
- cycle_13_2 (01/07/2013 - 31/08/2013)
- cycle_13_1 (02/05/2013 - 30/06/2013)
- cycle_12_5 (02/02/2013 - 01/05/2013)
- cycle_12_4 (11/11/2012 - 01/02/2013)
- cycle_12_3 (01/09/2012 - 10/11/2012)
- cycle_12_2 (01/07/2012 - 31/08/2012)
- cycle_12_1 (16/04/2012 - 30/06/2012)
- cycle_11_5 (16/01/2012 - 15/04/2012)
- cycle_11_4 (11/11/2011 - 15/01/2012)
- cycle_11_3 (11/08/2011 - 10/11/2011)
- cycle_11_2 (01/07/2011 - 10/08/2011)
- cycle_11_1 (17/05/2011 - 19/06/2011)
- cycle_10_3 (01/03/2011 - 16/05/2011)
- cycle_10_2 (22/06/2010 - 12/08/2010)
- cycle_10_1 (20/04/2010 - 28/05/2010)
- cycle_09_5 (16/02/2010 - 25/03/2010)
- cycle_09_4 (10/11/2009 - 21/12/2009)



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Filters

- **Investigation Type**
- **Instrument**

Apply

- ⊞ cycle_13_4 (11/11/2013 - 31/01/2013)
- ⊟ cycle_13_3 (01/09/2013 - 10/11/2013)
  - Dr Winfried Kockelmann et al; (2013): 1230027, STFC ISIS Facility.
  - ISIS; (2013): CAL_LOQ_2013-08-29T16:41:42, STFC ISIS Facility.
  - ISIS; (2013): CAL_PEARL_2013-08-12T18:54:55, STFC ISIS Facility.
  - ISIS; (2013): CAL_SANS2D_2013-08-28T15:26:21, STFC ISIS Facility.
  - ISIS; (2013): CAL_OFFSPEC_2013-09-06T16:01:53, STFC ISIS Facility.
  - ISIS; (2013): CAL_EMU_2013-08-07T12:08:16, STFC ISIS Facility.
  - Dr Dirk Visser et al; (2013): 1262009, STFC ISIS Facility, doi:10.5286/ISIS.E.24089719.
  - Dr Hazel Sparkes et al; (2013): 1310281, STFC ISIS Facility, doi:10.5286/ISIS.E.24090420.
  - Dr Sylvia McLain et al; (2012): 1200001, STFC ISIS Facility, doi:10.5286/ISIS.E.24089926.
  - Dr Tom Fennell et al; (2012): 1210213, STFC ISIS Facility, doi:10.5286/ISIS.E.24089599.
  - Dr James Lord et al; (2012): 1220055, STFC ISIS Facility, doi:10.5286/ISIS.E.24089615.
  - Dr Radu Coldea et al; (2012): 1210345, STFC ISIS Facility, doi:10.5286/ISIS.E.24088980.

investigations

- ⊞ cycle_13_2 (01/07/2013 - 31/08/2013)
- ⊞ cycle_13_1 (02/05/2013 - 30/06/2013)
- ⊞ cycle_12_5 (02/02/2013 - 01/05/2013)
- ⊞ cycle_12_4 (11/11/2012 - 01/02/2013)
- ⊞ cycle_12_3 (01/09/2012 - 10/11/2012)

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Filters

Investigation Type

- Disordered Materials Published Data
- calibration
- commercial_experiment
- engineering
- [x] experiment
- measurement
- simulation
- test

Instrument

Apply

- ⊞ cycle_13_4 (11/11/2013 - 31/01/2013)
- ⊟ cycle_13_3 (01/09/2013 - 10/11/2013)
  - Dr Dirk Visser et al; (2013): 1262009, STFC ISIS Facility, doi:10.5286/ISIS.E.24089719.
  - Dr Hazel Sparkes et al; (2013): 1310281, STFC ISIS Facility, doi:10.5286/ISIS.E.24090420.
  - Dr Sylvia McLain et al; (2012): 1200001, STFC ISIS Facility, doi:10.5286/ISIS.E.24089926.
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  - Dr James Lord et al; (2012): 1220055, STFC ISIS Facility, doi:10.5286/ISIS.E.24089615.
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- ⊞ cycle_12_5 (02/02/2013 - 01/05/2013)
- ⊞ cycle_12_4 (11/11/2012 - 01/02/20
- ⊞ cycle_12_3 (01/09/2012 - 10/11/20
- ⊞ cycle_12_2 (01/07/2012 - 31/08/20
- ⊞ cycle_12_1 (16/04/2012 - 30/06/20
- ⊞ cycle_11_5 (16/01/2012 - 15/04/2012)
- ⊞ cycle_11_4 (11/11/2011 - 15/01/2012)
- ⊞ cycle_11_3 (11/08/2011 - 10/11/2011)
- ⊞ cycle_11_2 (01/07/2011 - 10/08/2011)

filtered results

Filters are used to restrict results

Investigations are presented in the style of references

cycle_09_5 (16/02/2010 - 25/03/2010)

Professor John Evans; (2009): Magnetic and Structural Studies on Oxychalcogenides, STFC ISIS Facility.

Dr Diane Holland et al; (2009): Disorder in substituted beta-tricalcium phosphate for waste immobilisation, STFC ISIS Facility.

Dr Stuart Clarke; (2009): calcite water interface, STFC ISIS Facility.

Dr David Lennon et al; (2009): Evolutionary developments in the use of INS to investigate heterogeneous catalysts., STFC ISIS Facility.

Dr Ondrej Muransky et al; (2009): Continuation of Proposal (RB820197): The elasto-plastic response of dual-phase Zr-2.5Nb alloy using in-situ ND diffraction & EPSC modelling, STFC ISIS Facility.

Dr Ali Zarbakhsh et al; (2009): Surfactants at the metal-oil interface, STFC ISIS Facility.

Dr Gabriel Cuello; (2009): Absolute normalisation of spectra in DINS experiments:exploring the route to obtain scattering cross-sections, STFC ISIS Facility.

Dr Mark Johnson et al; (2009): A search for transverse phonons in DNA, STFC ISIS Facility.

Dr Matthew Tucker; (2009): Pressure-temperature phase diagram of of the Jahn-Teller transition in LaMnO3 , STFC ISIS Facility.

Dr Devashi Adroja et al; (2009): Inelastic neutron scattering investigations of the high temperature phase transition in YbAl3C3, STFC ISIS Facility.

Dr Abbie McLaughlin et al; (2009): The Crossover Between Giant Magnetoresistance and Superconductivity in RuSr2Gd1.8-xY0.2CexCu2O10-d , STFC ISIS Facility, doi:10.5286/ISIS.E.24078932.

Dr Howard Stone et al; (2009): Inter-phase load partitioning in a directionally-solidified Cr-Cr3Si eutectic, STFC ISIS Facility, doi:10.5286/ISIS.E.24078918.

Dr Winfried Kockelmann; (2009): Crystallographic determination of the minting of coins in Tudor Britain : an study of the Mary Rose collection. , STFC ISIS Facility.

Dr Matthias Gutmann et al; (2009): Diffuse scattering study of single crystal PrBa2Cu3O7-x, STFC ISIS Facility.

Dr Winfried Kockelmann; (2009): Combined imaging and diffraction studies of Renaissance bronzes , STFC ISIS Facility.

Dr Devashi Adroja et al; (2009): Experimental evidence for quadrupolar order in the heavy fermion compound Ce3Pd20Si6, STFC ISIS Facility.

Dr Devashi Adroja et al; (2009): Excitations in an orbitally dimerized spin S=1 honeycomb antiferromagnet, STFC ISIS Facility, doi:10.5286/ISIS.E.24077575.

unknown; (2009): 28/9-01 D2O + Pb 10t 80K, STFC ISIS Facility.

Dr Christophe Candolfi; (2009): Structural investigations of type-I clathrate compounds, STFC ISIS Facility.

unknown; (2009): μSR STUDY OF SPIN-FLUCTUATIONS IN ITINERANT METAMAGNETIC LACO9SI4, STFC ISIS Facility.

Professor Jon Goff et al; (2009): Divacancy superstructures and enhanced thermopower in NaxCayCoO2, STFC ISIS Facility, doi:10.5286/ISIS.E.24076930.

Dr Maria Paula Marques et al; (2009): THE CONFORMATIONAL BEHAVIOUR OF ANTIOXIDANT CHROMONES, STFC ISIS Facility.

Dr Graeme Blake et al; (2009): Crystal and magnetic structures of the anionogenic ferromagnet Ba0.85K0.15O2, STFC ISIS Facility, doi:10.5286/ISIS.E.24073785.

Dr Edward Oliver et al; (2009): Mg_sample5_-150deg_a;s-5;e0.00;p34.74, STFC ISIS Facility, doi:10.5286/ISIS.E.24071501.

Dr Matthias Gutmann; (2009): Neutron Diffraction Studies on CaCrFe3As3 compound, STFC ISIS Facility.

Science & Technology Facilities Council

ISIS Data Journal

The archive for ISIS research data

ISIS

Cycles | Investigation | Edit | Archived Versions

Previous Investigation | Next Investigation | Archive | Download

RB920302

Investigation title: Divacancy superstructures and enhanced thermopower in NaxCayCoO2

Release Date: 25-03-2013

Creator: *Professor Jon Goff*
Creator: *Professor Alan Tennant*
Creator: *Mr Manoj Soundhira Pandiyan*
Creator: *Dr Sivaperumal Uthayakumar*

DOI: 10.5286/ISIS.E.24076930

Date of Experiment: 22-09-2009 - 25-03-2010

Facility: ISIS Pulsed Neutron & Muon Source
Publisher: ISIS Data Journal

Data format: RAW/Nexus
Select the data format above to find out more about it.

Data Citation
The recommended format for citing this dataset in a research publication is as:
[author], [date], [title], [publisher], [doi]

For Example:
Professor Jon Goff et al; (2009): Divacancy superstructures and enhanced thermopower in NaxCayCoO2, STFC ISIS Facility, doi:10.5286/ISIS.E.24076930.

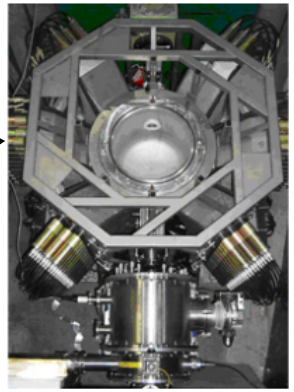
Abstract
Replacing Na ions in NaxCoO2 with divalent Ca ions results in the formation of ordered arrays of divacancy clusters, rather than the trivacancy clusters found for the pure compound at high x. Our previous experiment on SXD showed that Na0.7Ca0.1CoO2 adopts one of the superstructures with a low Coulombic ground state energy. We now wish to explore the ground states of the system doped with divalent Ca ions as a function of concentration in order to compare directly with theory. Doping with divalent ions results in a much lower hole concentration in the cobalt layers, and this is of fundamental interest since it will lead to new electronic and magnetic properties, and technological importance because it is expected to improve thermoelectric performance. We shall determine the ground states of NaxCayCoO2 with x+y=7/9, 11/13 and 13/15, where commensurate superstructures are predicted.

▶ **Additional Parameters**

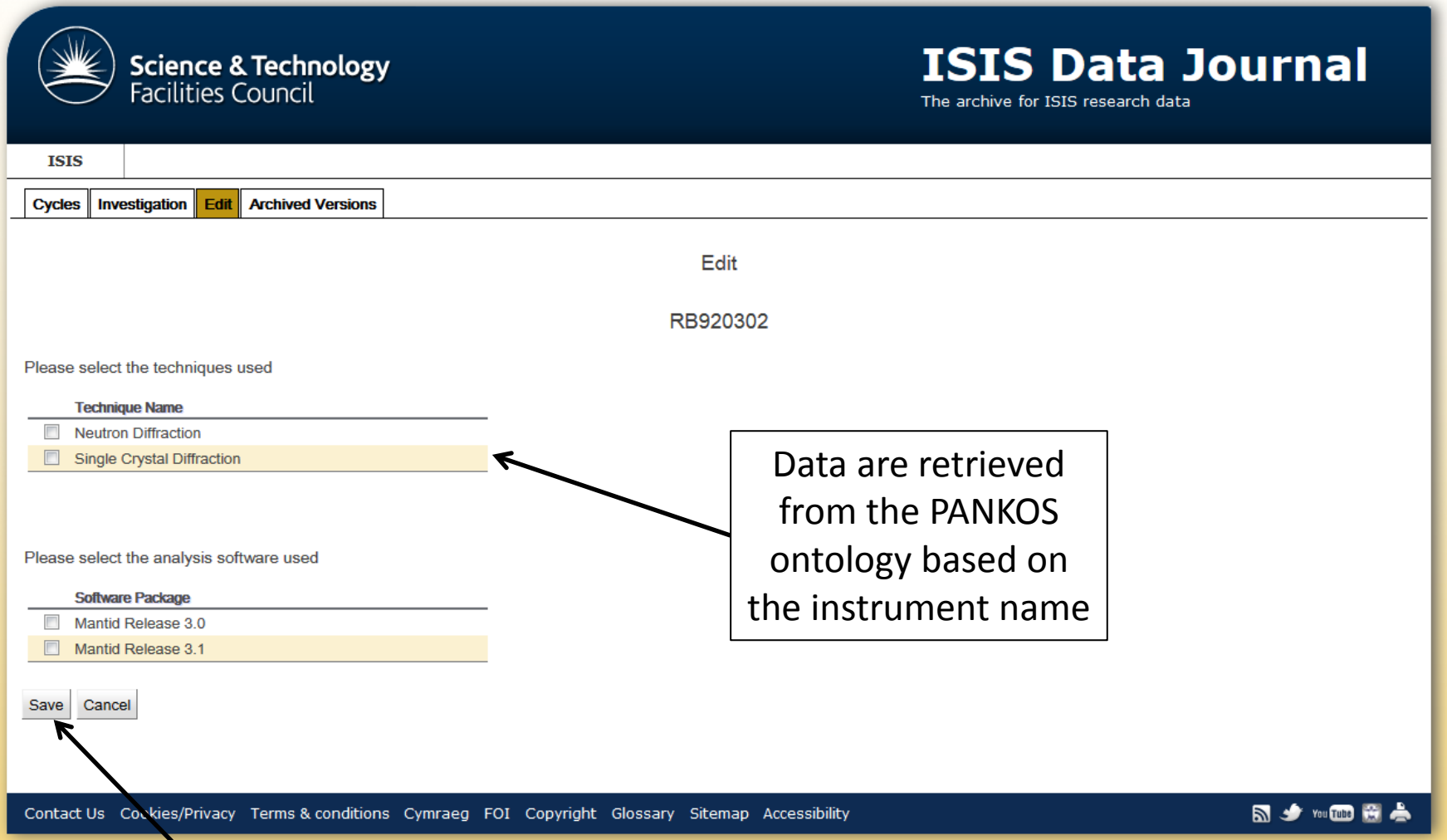
▶ **Data Sets**

Adding context

Details about an investigation are retrieved from the triple store



Data collected on the SXD instrument at the ISIS Pulsed Neutron & Muon Source facility



Data are retrieved from the PANKOS ontology based on the instrument name

Saving will create an annotation containing the URI of the ontology object.

Science & Technology Facilities Council

ISIS Data Journal

The archive for ISIS research data

ISIS

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RB920302

Investigation title: Divacancy superstructures and enhanced thermopower in NaxCayCoO2

Release Date: 25-03-2013

Creator: *Professor Jon Goff*
Creator: *Professor Alan Tennant*
Creator: *Mr Manoj Soundhira Pandiyan*
Creator: *Dr Sivaperumal Uthayakumar*

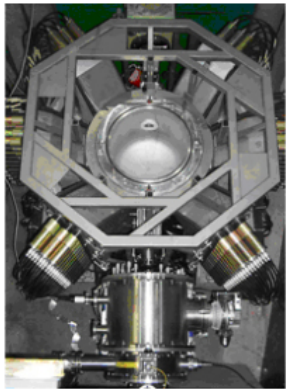
Creating SIP

DOI: 10.5286/ISIS.E.24076930

Date of Experiment: 22-09-2009 - 25-03-2010

Facility: ISIS Pulsed Neutron & Muon Source
Publisher: ISIS Data Journal

Data format: RAW/Nexus
Select the data format above to find out more about it.



Data collected on the SXD instrument at the ISIS Pulsed Neutron & Muon Source facility

Data Citation
The recommended format for citing this dataset in a research publication is as:
[author], [date], [title], [publisher], [doi]

For Example:
Professor Jon Goff et al; (2009): Divacancy superstructures and enhanced thermop … i:10.5286/ISIS.E.24076930.

Now contains merged data from the ontology

Abstract
Replacing Na ions in NaxCoO2 with divalent Ca ions results in the formation of orde … the trivacancy clusters found for the pure compound at high x. Our previous experiment on SXD showed that Na0.7Ca0.1CoO … w Coulombic ground state energy. We now wish to explore the ground states of the system doped with divalent Ca ions as a fu … rectly with theory. Doping with divalent ions results in a much lower hole concentration in the cobalt layers, and this is of fundamental interest since it will lead to new electronic and magnetic properties, and technological importance because it is expected to improve thermoelectric performance. We shall determine the ground states of NaxCayCoO2 with x+y=7/9, 11/13 and 13/15, where commensurate superstructures are predicted.

Techniques
Single Crystal Diffraction

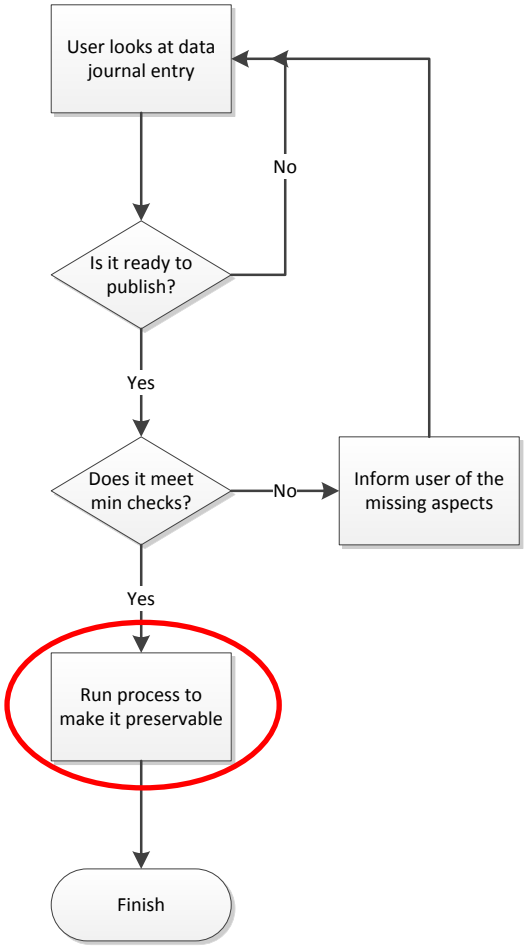
▶ **Additional Parameters**

▶ **Data Sets**

Preservation

User Initiated Preservation

This is the question that the creator of the experiment will ask



This work was partially supported by the SCAPE Project.
The SCAPE project is co-funded by the European Union under FP7 ICT-2009.4.1 (Grant Agreement number 270137).

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    <ns14:additionalAuthors>Mr Manoj Soundhira Pandiyan</ns14:additionalAuthors>
    <ns14:additionalAuthors>Professor Alan Tennant</ns14:additionalAuthors>
    <ns14:additionalAuthors>Dr Sivaperumal Uthayakumar</ns14:additionalAuthors>
    <ns14:summary>Replacing Na ions in NaxCoO2 with divalent Ca ions results in the formation of …. </ns14:summary>
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                <dc:creator>Holly Zhen</dc:creator>
                <dc:description>This ontology describes various neutron and synchrotron facilities from all over Europe, with
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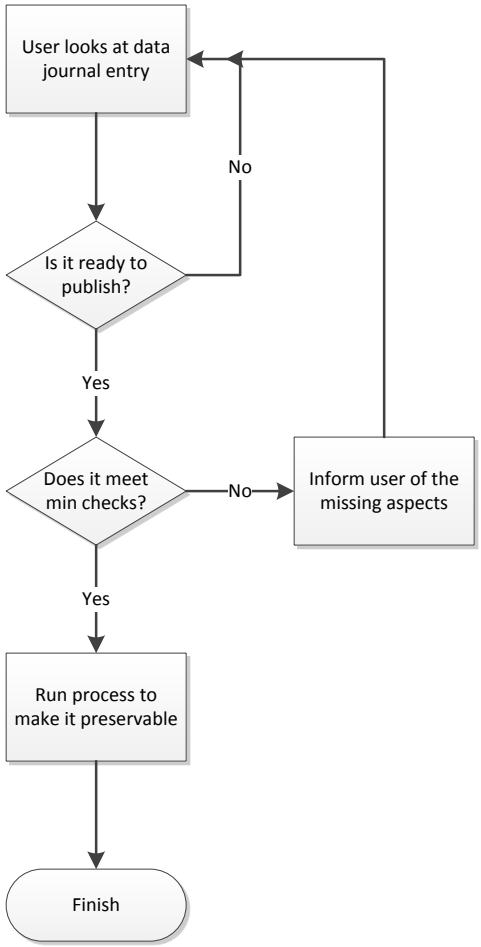
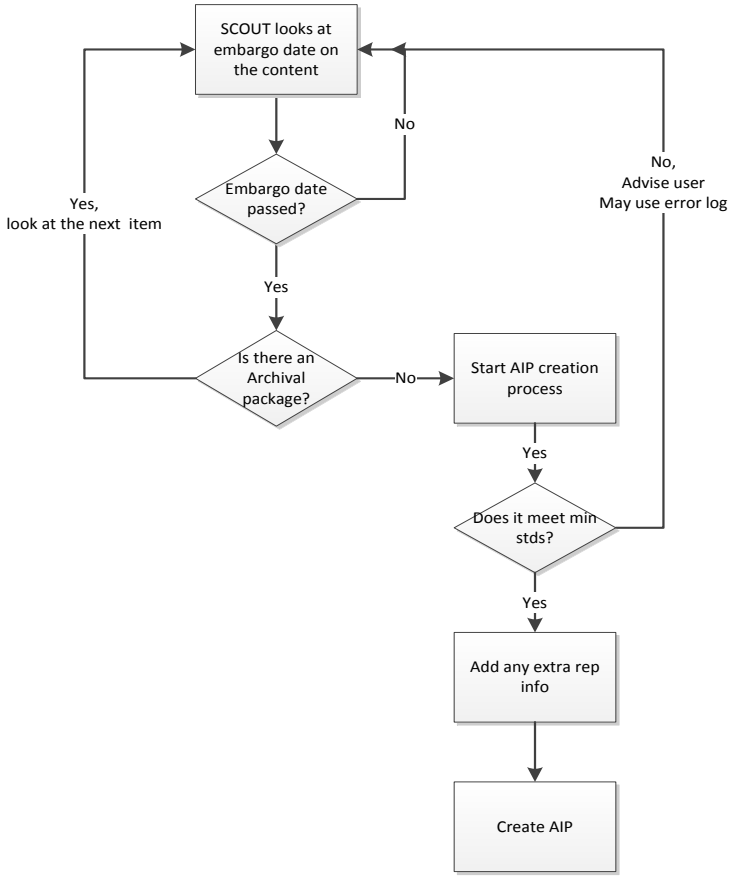
Automated Preservation

This is the question that the creator of the experiment will ask





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Hard Stuff….

- When is a Investigation Research Object Complete?
  - Does this change over time?
  - Does it changes depending on who you are?
- Preserving links – how much trust do you have in others?
  - What does this mean for the preserved object
- Is all data of the same value?
  - For ISIS data in SCAPE : should there be different processes for different investigation types, samples etc?

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Summary

- DONE
  - Initial IRO built from ICAT data
  - Links to ISIS web site automatically added
  - User may add links to PaNData ontology
  - User may add links to software packages
  - User may initiate archive process
  - IRO archived via SCAPE connector to Fedora repo
- What next
  - Add more data to archived IRO
  - Use SCOUT to automate triggering of archive process
  - Link in data from institutional repository

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