Mapping of metadata fields to possible NEXUS URIs. Note the NEXUS uris do not resolve. I have favored URIs in the NXxas group, but in many cases there is a more generic class that seems more appropriate for defining concepts when they can apply to any kind of experiment. In the ontology these are defined as owl:equivalentClass, so I use them.

Color explanation: different colors from different sources.

**NXxas:**

**NXxas\_new**

**XDI**

[uri from nexus ontology ] use prefix nxs for http://purl.org/nexusformat/definitions/

# **Fields**

Title [nxs:Field/NXentry/title]

start\_time [nxs:Field/NXentry/start\_time]

definition (profile = NXxas)(profile=NXxas\_new) [nxs:Field/NXentry/definition]

calculated [no uri?]

mode (XAS measurement mode) [nxs:Field/NXxas/ENTRY/DATA/mode]

name: (controlled list of process being monitored to obtain the spectrum.

element XD**I**

symbol []

edge XDI (controlled list) []

Instrument []

CalibrationDescription (ExPANds) [nxs: Group/NXdetector/calibration\_method]

Configuration (Daphne) [nxs:Group/NXentry/experiment\_documentation]

installed options, (Daphne)

name [nxs:Field/NXinstrument/name]

source []

type [nxs:Field/NXsource/type]

name [nxs:Field/NXsource/name]

probe (constant= ‘x-ray) [nxs:Field/NXsource/probe]

monochromator []

name []

crystal [nxs:Field/NXcrystal/chemical\_formula]

type [nxs:Field/NXcrystal/type]

reflection [nxs:Field/NXcrystal/reflection]

d-spacing [nxs:Field/NXcrystal/d\_spacing]

beamline []

name []

collimation []

focusing []

harmonic\_rejection []

detector (used to hold data…) What is difference between detector and monitor?

monitor (not in NXxas\_new) (like detector)

mode (monitor or timer) [nxs:Field/NXmonitor/mode]

preset [nxs: Field/NXmonitor/preset]

type (‘detector.i0’) how the incident flux was measured

detector.it, if, ir – descriptions of how fluxes were measured

Sample [use iSamples URI?]

Name [nxs:Field/NXsample/name]

Identifier []

stoichiometry (chemical formula) [nxs:Field/NXsample/chemical\_formula]

sample preparation []

temperature (or other environmental conditions….) [nxs:Field/NXsample/temperature] or stress\_field, electric\_field, pressure, magnetic\_field, density, concentration.

size (sample property) (Daphne) [nxs:Field/NXsample/mass, nxs:Field/NXsample/thickness]

crystalStructure (Daphne) [nxs:Field/NXsample/point\_group] or space\_group

materialUnitCell (Daphne) [ nxs:Field/NXsample/unit\_cell]

parentSample (Daphne) []

state (Daphne) []

Process (data processing description) TBD

wasGeneratedBy, @type=DataProcessing (ExPANds)

Software package information (input,output, functions, etc.) (ExPANds)

Dependence tracking (ExPANds)

workflow (ExPANds)

Collection (Apparently an array of all the data; is Nxscan in some data instances)

columns – array lists columns in raw data array

start\_time [nxs:Field/NXentry/start\_time]

end\_time [nxs:Field/NXentry/end\_time]

data\_collector

name [nxs:Field/NXuser/name]

orcid [nxs:Field/NXuser/ORCID]

role [nxs:Field/NXuser/role]

experimenters (operators) see above

Facility []

name

energy [] facility property or instrument property?

current [] facility property or instrument property?

x-ray source [nxs:Field/NXsource/type]

# Variables:

From list of column labels in xdi

Prefix: nxs: <http://purl.org/nexusformat/definitions/>

|  |  |  |  |
| --- | --- | --- | --- |
| **Column label** | **Meaning** | **URI** | **choice of units** |
| **cdi:name and schema:name** | **schema:alternateName** |  | **schema:unitText and cdi:simpleUnitOfMeasure** |
| energy | mono energy | nxs:Field/NXmonochromator/energy | eV / keV / pixel. nxs: Units/NX\_ENERGY |
| energy\_error |  | nxs: Field/NXmonochromator/energy\_error | nxs: Units/NX\_ENERGY |
| angle | mono angle | -- | degrees / radians / steps |
| i0 | monitor intensity | nxs: Field/NXxas/ENTRY/MONITOR/data |  |
| itrans | transmission intensity | nxs: Field/NXxas/ENTRY/INSTRUMENT/absorbed\_beam/data |  |
| ifluor | fluorescence intensity | nxs: Field/NXfluo/entry/INSTRUMENT/fluorescence/data (??) |  |
| irefer | reference intensity | -- |  |
| mutrans | mu transmission | -- |  |
| mufluor | mu fluorescence | -- |  |
| murefer | mu reference | -- |  |
| normtrans | normalized mu transmission | -- |  |
| normfluor | normalized mu fluorescence | -- |  |
| normrefer | normalized mu reference | -- |  |
| k | wavenumber | -- | nxs: Units/NX\_WAVENUMBER |
| chi | EXAFS |  |  |
| chi\_mag | magnitude of Filtered chi(k) |  |  |
| chi\_pha | phase of Filtered chi(k) |  |  |
| chi\_re | real part of Filtered chi(k) |  |  |
| chi\_im | imaginary part of Filtered chi(k) |  |  |
| r | radial distance |  |  |
| chir\_mag | magnitude of FT[chi(k)] |  |  |
| chir\_pha | phase of FT[chi(k)] |  |  |
| chir\_re | real part of FT[chi(k)] |  |  |
| chir\_im | imaginary part of FT[chi(k)] |  |  |

# Notes

Compilation of information about data collected w.r.t. XAS experiment

From examples (namespace is a placeholder...)

Conceptual Variables

xas:absorptionCoefficientConcept

xas:fluorescenceAbsorptionCoefficientConcept

xas:transmittedIntensityConcept

xas:incidentIntensityConcept

xas:monochromatorEnergyConcept

Properties

xas:collimation

xas:focusing

xas:harmonic\_rejection

xas:d\_spacing

xas:fluxMeasureMethod

xas:pressure (experiment environment)

xas:edge\_energy

xas:energy

xas:xray\_source

xas:porosity (sample)

xas:stoichiometry (composition of sample)

xas:sample.prep (sample)

Entities

xas:AnalysisEvent

xas:Instrument

xas:Beamline

xas:Monochromator

xas:Detector

xas:Facility

xas:xdiCDIF -- uri for cdif xas profile for dcterms:conformsTo.

prov:wasGeneratedBy-- extend usage to include 'AnalysisEvent', with instrument, sample (mainEntity), Facility(location), dates, operators, additionalProperty.... Extend to include 'DataProcessing' with description of software, workflow, actors...

From Daphne

contributor roles: {operator, Principal Investigator,Co-Proposers,Experimental team, Facility, pointOfContact,

instrument -- configuration, installed options,

analysisEvent-- Environmental conditions (XDI has a list...)

sample -- state (values look like iSamples material object type)

xas:size (sample property)

xas:crystalStructure

xas:materialUnitCell

parentSample

ExPANds

contributor roles: proposal author, roles in processing if include wasGeneratedBy, @type=DataProcessing

instrument -- calibrationDescription, other parameters??

link to lab notebook??

wasGeneratedBy, @type=DataProcessing

Software package information (input,output, functions, etc.)

Dependence tracking

workflow