# Annotated species XML schema (file species.xsd)

Version 2015-05-20

The quantum-simulation.org species XML Schema defines the allowed content of species documents according to the http://www.quantum-simulation.org specification. Validating XML parsers (such as Apache Xerces-C) use the XML Schema file “species.xsd” to verify the correctness of species documents.

## *XML header*

```
<?xml version="1.0"?>
<schema xmlns="http://www.w3.org/2001/XMLSchema"
  targetNamespace="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0"
  xmlns:fpmd="http://www.quantum-simulation.org/ns/fpmd/fpmd-1.0">

  <annotation>
    <documentation>
      version 2015-05-20
      http://www.quantum-simulation.org
      FPMD atomic species XML Schema specification.
      Copyright (c) 2006-2014 The Regents of the University of California.
    </documentation>
  </annotation>
```

The header section contains the XML declaration of the `<schema>` element and the definition of the XMLSchema and fpmd namespaces. The `<annotation>` section describes the version of the species Schema specification. The current version is `2015-05-20` .

## *<species> element*

```
  <element name="species" type="fpmd:speciesType"/>
  <complexType name="speciesType">
    <sequence minOccurs="0">
      <element name="description" type="string" minOccurs="0"
       maxOccurs="1"/>
      <element name="symbol" type="NMTOKEN"/>
      <element name="atomic_number" type="nonNegativeInteger"/>
      <element name="mass" type="fpmd:positiveDouble"/>
      <choice>
        <element name="norm_conserving_pseudopotential"
          type="fpmd:norm_conserving_pseudopotentialType"/>
        <element name="norm_conserving_semilocal_pseudopotential"
          type="fpmd:norm_conserving_semilocal_pseudopotentialType"/>
      </choice>
    </sequence>
    <attribute name="name" type="NMTOKEN" use="optional"/>
    <attribute name="href" type="anyURI" use="optional"/>
  </complexType>
```

The `<species>` element consists of a `<description>` element, a `<symbol>` element, an `<atomic_number>`, a `<mass>` element and an optional `<norm_conserving_pseudopotential>` or `<norm_conserving_semilocal_pseudopotential>` element.
This allows for the description of atoms using different types of pseudopotentials. Other element types can be added to include the representation of atoms using other types of pseudopotentials, or possibly classical force fields. The `<species>` element has a name attribute that is used by an application to

refer to the species. A <species> element can also have an href attribute that refers to a species definition given by a URI. This allows for two different uses of the <species> element, which we refer to as “definition” and “declaration” of a <species>.

## Definition of a species

When used in a standalone file defining the species, the name attribute and the href attribute of the <species> element should not be defined. The rest of the <species> element must be present.

## Declaration of a species

In a sample document, a <species> element may be included in two different ways:

1. The <species> element contains a complete definition. The name attribute should be defined for the application to associate the <species> element with that name.
2. The href attribute contains the URI of a document in which the <species> element is defined. In that case, the body of the <species> element should be empty. Applications can use the href attribute to access the species definition via the given URI, using e.g. a web-enabled XML parser.

The <symbol> element contains the two-character symbol of the element as it appears in the Periodic Table. This can be used by applications to recognize the element and assign it some other characteristics, such as e.g. color or ball radius for visualization purposes. The <mass> element must contain the mass in units in which the mass of carbon is 12.

### *norm_conserving_pseudopotentialType definition*

```
<complexType name="norm_conserving_pseudopotentialType">
  <sequence>
    <element name="valence_charge" type="nonNegativeInteger"/>
    <element name="lmax" type="nonNegativeInteger"/>
    <element name="llocal" type="nonNegativeInteger"/>
    <element name="nquad" type="nonNegativeInteger"/>
    <element name="rquad" type="fpmd:nonNegativeDouble"/>
    <element name="mesh_spacing" type="fpmd:positiveDouble"/>
    <element name="core_density" minOccurs="0" maxOccurs="1">
      <complexType>
        <simpleContent>
          <extension base="fpmd:doubleListType">
            <attribute name="size" type="positiveInteger" use="required"/>
          </extension>
        </simpleContent>
      </complexType>
    </element>
    <element name="projector" minOccurs="1" maxOccurs="unbounded">
      <complexType>
        <sequence>
          <element name="radial_potential" type="fpmd:doubleListType"/>
          <element name="radial_function" minOccurs="0"
            type="fpmd:doubleListType"/>
        </sequence>
        <attribute name="l" type="nonNegativeInteger" use="required"/>
        <attribute name="size" type="positiveInteger" use="required"/>
      </complexType>
    </element>
  </sequence>
</complexType>
```

A <norm_conserving_pseudopotential> element is defined by the following elements

<valence_charge> Number of valence electrons

<lmax> Largest angular momentum included in the potential

<llocal> Angular momentum taken to be local

<nquad> Number of quadrature points used in the radial integration for semi-local potentials. If *nquad*=0, the Kleinman-Bylander form is assumed. If *nquad*>0, a set of *nquad* equally spaced points in the interval [0,rquad] is used for radial integration of semi-local projectors.

<rquad> Endpoint $r_c$ of the interval for radial integration of semi-local projectors. The value of <rquad> must be chosen so that all potentials $v_l(r)$ for all angular momenta are equal beyond r=rquad.

<mesh_spacing> Spacing of the linear radial grid $\{r_i\}$ on which projectors and radial functions are defined. Functions defined on the radial grid are given as a list of values $f(r_i)$ starting at $r_0=0$ .

<core_density> A function describing the core charge density for use in non-linear core corrections.

For each angular momentum, a <projector> element must be defined. Each <projector> consists of a <radial_potential> function describing the potential $v_l(r)$ for that angular momentum, and a <radial_function> describing the atomic orbital $\phi_l(r)$ for that projector. The l attribute defines the angular momentum of the projector, and the size attribute defines the number of points in the linear radial mesh.

If nquad = 0, the non-local potential operator has the Kleinman-Bylander separable form

$$\hat{V}\,\psi(r,\theta,\varphi)=v_{l_{\text{local}}}(r)\,\psi(r,\theta,\varphi)+$$
$$\sum_{l=0,\,l\neq l_{\text{local}}}^{l_{\max}}\frac{1}{I_l}\sum_{m=-1}^{l}\delta v_l(r)\,\phi_l(r)\,Y_l^m(\theta,\varphi)\int_0^{\infty}\delta v_l(r')\,\phi_l(r')\,Y_l^m(\theta',\varphi')\,\psi(r',\theta',\varphi')\,r'^2\,dr'\sin\theta'\,d\theta'\,d\varphi'$$

where

$$\delta v_l(r)=\left[v_l(r)-v_{l_{\text{local}}}(r)\right]$$

and

$$I_l=\int_0^{\infty}\phi_l(r)\,\delta v_l(r)\,\phi_l(r)\,r^2\,dr$$

If nquad > 0, the potential operator has the semi-local form

$$\hat{V}\,\psi(r,\theta,\varphi)=v_{l_{\text{local}}}(r)\psi(r,\theta,\varphi)$$
$$+h\sum_{i=0}^{n_{\text{quad}}}4\pi r_i^2\sum_{l=0,l\neq l_{\text{local}}}^{l_{\max}}\sum_{m=-1}^{l}Y_l^m(\theta,\varphi)\,\delta v_l(r)\,\delta(r-r_i)\int_0^{\infty}Y_l^m(\theta',\varphi')\,\psi(r_i,\theta',\varphi')\sin\theta'\,d\theta'\,d\varphi'$$

where $h=r_c/n_{\text{quad}}$ and $r_i=i\,h$

Note that a local potential is a special case of <norm_conserving_pseudopotential> in which lmax=0 and llocal = 0. A local potential only includes a single projector.

## *norm_conserving_semilocal_pseudopotentialType definition*

```
<complexType name="norm_conserving_semilocal_pseudopotentialType">
  <sequence>
    <element name="valence_charge" type="nonNegativeInteger"/>
    <element name="mesh_spacing" type="fpmd:positiveDouble"/>
    <element name="core_density" minOccurs="0" maxOccurs="1">
      <complexType>
        <simpleContent>
          <extension base="fpmd:doubleListType">
            <attribute name="size" type="positiveInteger" use="required"/>
          </extension>
        </simpleContent>
      </complexType>
    </element>
    <element name="local_potential">
      <complexType>
        <simpleContent>
          <extension base="fpmd:doubleListType">
            <attribute name="size" type="positiveInteger" use="required"/>
          </extension>
        </simpleContent>
      </complexType>
    </element>
    <element name="projector" minOccurs="0" maxOccurs="unbounded">
      <complexType>
        <simpleContent>
          <extension base="fpmd:doubleListType">
            <attribute name="l" type="nonNegativeInteger" use="required"/>
            <attribute name="i" type="nonNegativeInteger" use="required"/>
            <attribute name="size" type="positiveInteger" use="required"/>
          </extension>
        </simpleContent>
      </complexType>
    </element>
    <element name="d_ij" minOccurs="0" maxOccurs="unbounded">
      <complexType>
        <simpleContent>
          <extension base="double">
            <attribute name="l" type="nonNegativeInteger" use="required"/>
            <attribute name="i" type="nonNegativeInteger" use="required"/>
            <attribute name="j" type="nonNegativeInteger" use="required"/>
          </extension>
        </simpleContent>
      </complexType>
    </element>
  </sequence>
</complexType>
```

A <norm_conserving_semilocal_pseudopotential> element represents a norm-conserving pseudpotential with an arbitrary number of projectors per angular momentum. It is defined by the following elements:

<valence_charge> Number of valence electrons

<mesh_spacing> Spacing of the linear radial grid $\{r_i\}$ on which projectors and other functions are defined. Functions defined on the radial grid are given as a list of values $f(r_i)$ starting at $r_0=0$ .

<core_density> A function describing the core charge density for use in non-linear core corrections.

<local_potential> Local potential $v_{\text{local}}(r)$ .

<projector> Projector $\chi_{li}(r)$ . The attributes are the index i of the projector and its angular momentum l. The size attribute is the number of points on which the projector is defined.

<d_ij> Matrix element $D^l_{ij}$ . The attributes are the indices i and j of the associated projectors and their angular momentum l.

The potential has the form

$$\hat{V}\psi(r,\theta,\varphi)=v_{\text{local}}(r)\psi(r,\theta,\varphi)+$$
$$\sum_{i,j}\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{l}\chi_{li}(r)Y_l^m(\theta,\varphi)D^l_{ij}\int\chi_{lj}(r')Y_l^m(\theta',\varphi')\psi(r',\theta',\varphi')\,4\pi r'^2\,dr'\sin\theta'\,d\theta'\,d\phi'$$

where $D^l=(B^l)^{-1}$ and

$$B^l_{ij}=4\pi\int_0^\infty\phi_{li}(r)\chi_{lj}(r)\,r^2\,dr$$

as defined in D. R. Hamann, Phys. Rev. B 88 , 085117 (2013).

## *Miscellaneous*

```
  <simpleType name="doubleListType">
    <list itemType="double"/>
  </simpleType>

  <simpleType name="positiveDouble">
    <restriction base="double">
      <minExclusive value="0"/>
    </restriction>
  </simpleType>

  <simpleType name="nonNegativeDouble">
    <restriction base="double">
      <minInclusive value="0"/>
    </restriction>
  </simpleType>

</schema>
```