Annotated species XML schema (file species.xsd)

The 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> $Id: species.xsd,v 1.6 2008/03/07 20:05:31 fgygi Exp $
      http://www.quantum-simulation.org
      FPMD atomic species XML Schema specification.
      Copyright (c) 2006-2008 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. In the present example, the version is 1.6.

<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"/>
      <element name="norm_conserving_pseudopotential" minOccurs="0"
       maxOccurs="1"
       type="fpmd:norm_conserving_pseudopotentialType"/>
    </sequence>
    <attribute name="name" type="NMTOKEN" use="optional"/>
    <attribute name="href" type="anyURI" use="optional"/>
  </complexType>
```

A <species> element consists of a <description> element, a <symbol> element, an <atomic_number>, a <mass> element and an optional <norm_conserving_pseudopotential> element. This allows for the description of atoms within different approximations. Other element types can be added to include the representation of atoms using other types of pseudopotentials, or possibly classical force fields. A <species> has a name attribute that is used by an application to refer to the species. A <species> 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 file defining the species, the name attribute of the <species> element must be defined and the href attribute should not be defined. The rest of the <species> element must be present.

Declaration of a species

A <species> element can be used to declare a species without giving its full definition. This is the case for instance when a <species> is mentioned in the body of a <sample> element. In that case, the name attribute of the species should not be present, but the href attributed should be used to point to the document in which the <species> is defined. In that case, the body of the <species> element is empty.

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="projector" minOccurs="1" maxOccurs="unbounded">
        <complexType>
          <sequence>
            <element name="radial_potential">
              <simpleType>
                <list itemType="double"/>
              </simpleType>
            </element>
            <element name="radial_function" minOccurs="0">
              <simpleType>
                <list itemType="double"/>
              </simpleType>
            </element>
          </sequence>
          <attribute name="l" type="nonNegativeInteger" use="required"/>
          <attribute name="size" type="positiveInteger" use="required"/>
        </complexType>
      </element>
    </sequence>
  </complexType>

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

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

```
    </restriction>
  </simpleType>
```

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>	The endpoint of the interval for radial integration of semi-local projectors. The value of <rquad> must be chosen so that all potentials for all angular momenta are equal beyond r=rquad.
<mesh_spacing>	The spacing of the linear radial grid on which projectors are defined.

For each angular momentum, a <projector> element must be defined. Each <projector> consists of a <radial_potential> describing the potential for that angular momentum, and a <radial_function> describing the atomic orbital 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.

```
</schema>
```