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XML Tools for First-Principles Molecular Dynamics Simulations[1]

FRANCOIS GYGI, University of California Davis — We present a set of XML Schema specifications for the representation of electronic structure data and first-principles molecular dynamics (FPMD) simulation data. The schemas (available at http://www.quantum-simulation.org) include the description of FPMD simulation samples and pseudopotentials in an extensible and code-neutral way. Automatic validation of simulation samples can be achieved using publicly available XML parsers such as Apache Xerces-C. We present examples of web-based remote collaboration in which simulation samples and pseudopotentials are accessed using the http protocol. Data analysis using XSLT scripts and a visualization program for remote inspection of simulation samples will also be demonstrated.

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