Abstract Submitted
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An XML-based framework for the validation and verification of electronic structure codes[1] GARY YUAN, FRANCOIS GYGI, University of California Davis — The process of validation and verification of the results of electronic structure calculations involves comparisons of data sets obtained with widely disparate software packages, including a large diversity of data formats. We present a web-based framework aimed at facilitating automatic comparison between electronic structure computation results and first-principles molecular dynamics simulations. The framework makes extensive use of XML in the representation and translation of data sets. An application to the automatic verification of results obtained with the Qbox first-principle simulation code (http://eslab.ucdavis.edu/software/qbox) and the Quantum Espresso code (http://quantum-espresso.org) will be presented

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