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### **New Tools for the Verification and Validation of Electronic Structure Calculations<sup>1</sup>**

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First-principles electronic structure calculations are playing an increasingly important role in the prediction of materials properties and in the interpretation of experimental data. Numerous simulation codes including various levels of approximations and various numerical approaches are now readily available to users. The complexity of first-principles calculations and the large number of input parameters needed in a simulation make it challenging to obtain high quality, reproducible data. Results obtained with different electronic structure codes are difficult to compare as they involve a multitude of data formats, making the process of verification and validation (V&V) of electronic structure data complex and error prone. In order to facilitate V&V activities, we have introduced ESTEST [1,2], a web-based framework that allows for automatic comparison and post-processing of results obtained with six electronic structure codes. Recent developments make it possible to extend this functionality to a decentralized network of servers. We discuss general issues related to the process of verification and validation of electronic structure data and outline requirements for the development of future V&V tools.

[1] G. Yuan and F. Gygi, Computational Science & Discovery 3, 015004 (2010) doi:10.1088/1749-4699/3/1/015004G

[2] <http://estest.ucdavis.edu>

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