NIST Interatomic Potential Repository: Tools for Improved Selection, Use, and Creation of Interatomic Potentials

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ABSTRACT

The MGI seeks to significantly decrease the cost and time of development and integration of new materials. Within the domain of atomistic simulations, several roadblocks stand in the way of reaching this goal. While the NIST Interatomic Potentials Repository hosts numerous interatomic potentials (force fields), researchers cannot immediately determine the best choice(s) for their use case. Researchers developing new potentials lack a comprehensive portfolio of efficient tools capable of calculating and archiving the properties of their potentials. This project has expanded its scope to address these needs via new effort within three thrust areas: (i) development of reusable property calculation tools, (ii) exemplary adoption of open data mechanisms, and (iii) development of comprehensive and interactive data visualization tools. These new resources will reduce the time required to select an existing interatomic potential for a specific use case and help others (such as the private sector) develop new interatomic potentials using efficient property calculation tools.