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Computational Catalysis: Creating a User-Friendly Tool for Research and Education

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ABSTRACT

Catalysis is used in a significant portion of production processes in the industrialized world, including most processing of chemicals and fuels. This makes maximizing the efficiency of catalysts a high priority. However, the immense number of candidates for new catalysts precludes the possibility of testing all of them by experiments. Density functional theory (DFT) has been widely and successfully used to calculate material properties relevant to catalysis and to screen promising candidates for experimental testing, but there currently exists no publicly-available, user-friendly tool for performing these DFT calculations. This work details the development of such a tool for nanoHUB.org using Quantum Espresso and the Atomic Simulation Environment Python library. Testing was performed for a variety of preloaded structures and surfaces to determine the optimal input values for achieving accurate results in minimal time. The tool's capabilities were evaluated by benchmarking its results against those of previous computational work. The close agreement of these results indicates the readiness of the tool for use in research, and the user interface will enable its use in education to teach students about catalysis and to inspire the next generation of researchers in the field.

KEYWORDS

computational catalysis, catalyst design, heterogeneous catalysis, simulation, density functional theory