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Extending Quantum Simulations to Long Timescales for Materials Under Reactive Conditions

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Knowledge of the equation of state and chemical kinetics of materials under reactive conditions is needed for a wide number of research areas, including studies of planetary interiors, astrobiology, high-pressure materials synthesis, and material corrosion. In this regard, we have developed a family of classical and semi-empirical quantum simulation methods which leverage the accuracy of Kohn-Sham Density Functional Theory (DFT) while yielding several orders of magnitude increase in computational efficiency. This allows for direct simulation of many different types of experiments, where chemical events can equilibrate on timescales that are orders of magnitude longer than can be achieved with standard quantum approaches.

Here, we present several different applications of our models, including mechano-chemical synthesis of semi-conducting diamonds, corrosion on actinide metal surfaces, and the shock synthesis of life building molecules in impacting astrophysical ices. Our methods provide a straightforward way to conduct computationally efficient quantum simulations over a broad range of conditions, where physical and chemical properties can be difficult to interrogate directly and there is historically a significant reliance on theoretical approaches for interpretation and validation of experimental results.