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Research Article

Phase Transition in Silicon from Machine Learning Informed Metadynamics

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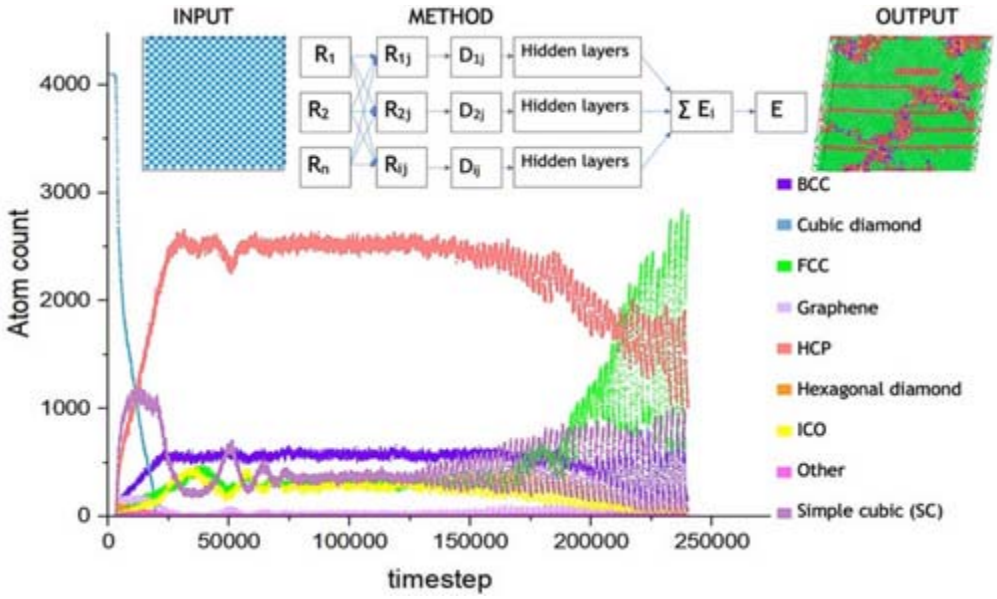
Graphical Abstract

The article reveals the phase transition in a system of 4096 Silicon atoms from cubic diamond to a concluding amalgam of FCC and HCP phases with the use of machine learning potentials (MLP) built from the deep neural network (DNN) mechanism. The Deep Potential is constructed by training on extensive ab initio datasets depicting the behavior of the system under 25 GPa.



Abstract

Investigating reconstructive phase transitions in large-sized systems requires a highly efficient computational framework with computational cost proportional to the system size. Traditionally, widely used frameworks such as density functional theory (DFT) have been prohibitively expensive for extensive simulations on large systems that require long-time scales. To address this challenge, this study employed well-trained machine learning potential to simulate phase transitions in a large-size system. This work integrates the metadynamics simulation approach with machine learning potential, specifically deep potential, to enhance computational efficiency and accelerate the study of phase transition and consequent development of grains and dislocation defects in a system. The new method is demonstrated using the phase transitions of bulk silicon under high pressure. This approach has revealed the transition path and formation of polycrystalline silicon systems under specific stress conditions, demonstrating the effectiveness of deep potential-driven metadynamics simulations in gaining insights into complex material behaviors in large-sized systems.

Conflict of interests

The authors declare no conflict of interest.

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Front Cover:

Michal Bajdich and co-workers

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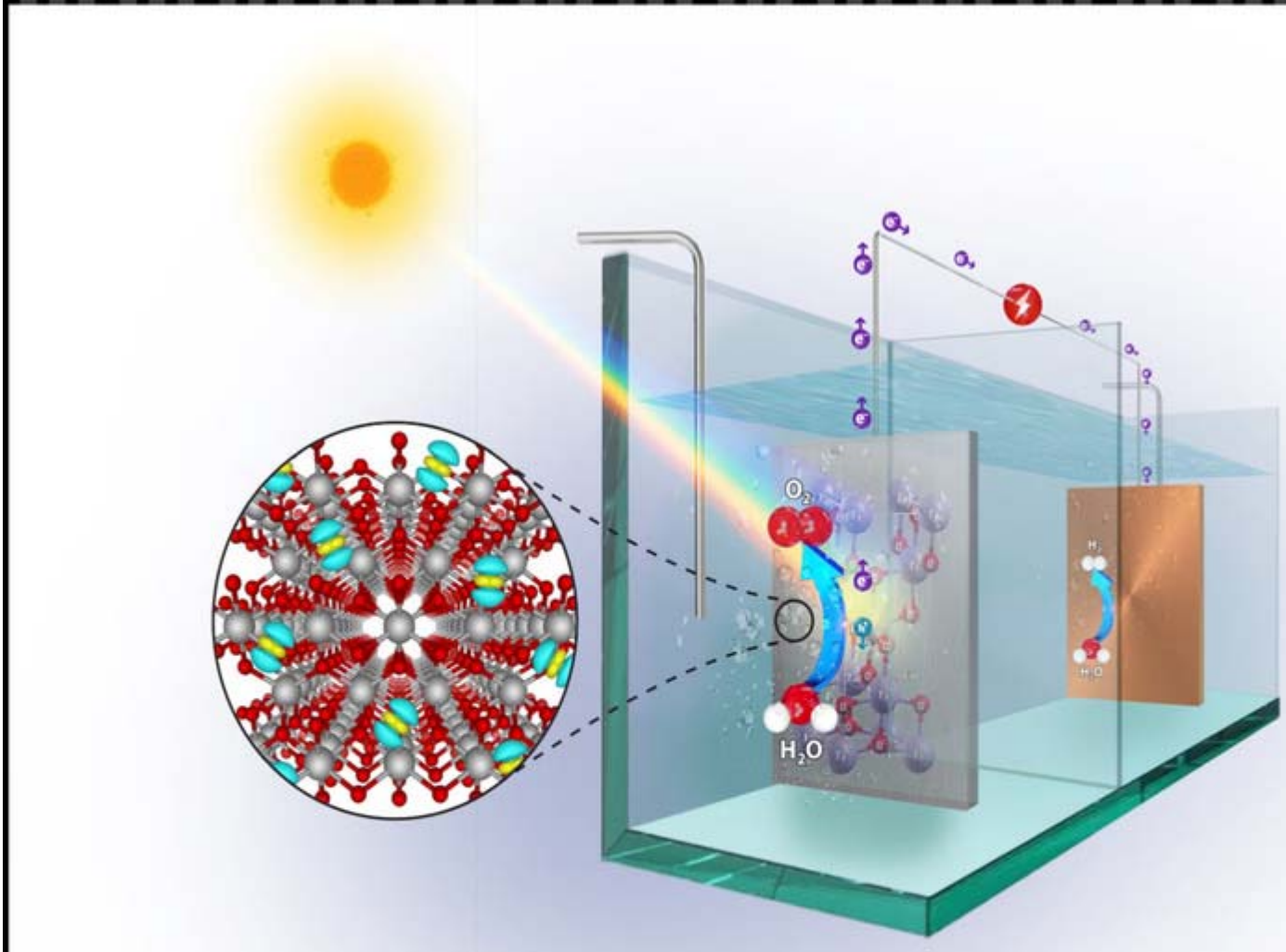

Early View

Online Version of Record before inclusion in an issue

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