Development of Graph Neural Network Interatomic Potential to Investigate Diamond Oxidation, Graphitization, and Wear

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Purpose	Investigate the Mechanism of Diamond Oxidation, Graphitization and Wear Using GNN Molecular Dynamics
Outline	Develop Interatomic Potential, Perform Simulations, Analyze Results and Develop Atomic and Quantum-Level Theory
Results	Elucidated Diamond Surface Facet-Dependent Properties
	Discover Graphitization Suppression and Control Method
	Propose Novel Graphene on Diamond Fabrication Method
	Develop Computational Tools for Machine Learning MD Reliability Estimation, Wear Analysis and Structure Identification, and Chemical Reaction Saddle Point Search

Computing system:	SQUID General Purpose CPU and GPU nodes
CPU node-hour	91,000 node-hour
GPU node-hour	5,000 node-hour

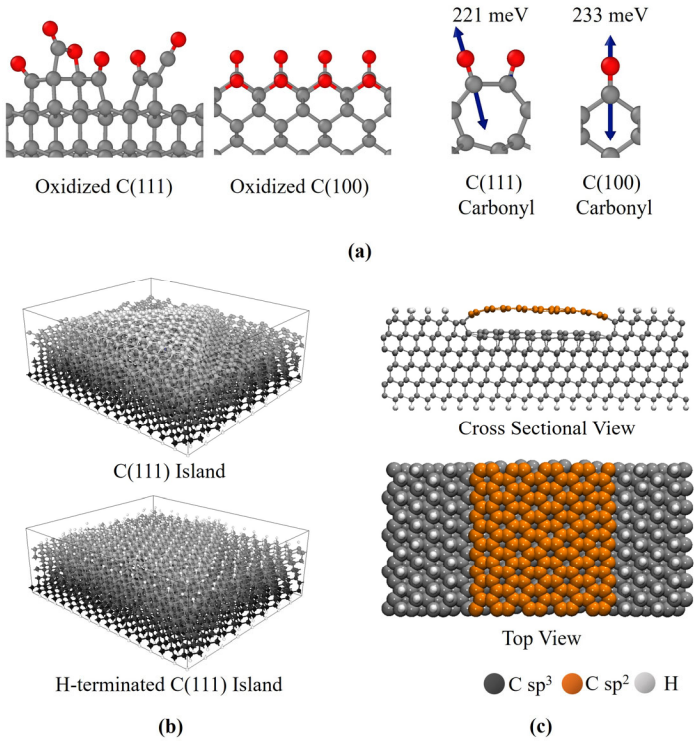

Fig. 1. Quantum engineering and design of diamond material using first principles and machine learning molecular dynamics simulations. (a) oxidation, (b) graphitization suppression, and (c) epitaxial graphene self assembly.