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A Feasibility Study for Quantum Computing Methodologies in Automotive Advanced Material Investigation

- Molecular Dynamics Study for Liquid Hydrogen using Quantum Gate Simulator -

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Regarding the calculation methodologies for future high performance computing (HPC) in variety of automotive research, quantum computing technologies are one of the promising candidate that could potentially instead conventional multi-core super computers. The functional material design, that idealize high performance electric vehicle or fuel cell electric vehicle, would be a suitable target for this novel HPC technologies.

In this article, for the purpose of elucidating the practical possibility of quantum computer algorithms in future, we apply quantum gate simulations combining with classical molecular dynamics modelling to reproduce thermodynamic behavior of molecular composite materials. (Quantum gate simulator is as the exact simulator of quantum computer gate operation with no harmful quantum noise in limited small sized systems.)

Liquid hydrogen, a potential candidate for hydrogen storage, are studied as the simplest case of this benchmark. Notable quantitative improvements of prediction performance in molecular dynamics modelling are obtained. This denotes quantum computing methodologies for multi body electron systems (e.g. VQE, variational quantum eigen solver) would be useful as the 'forcefield generator tool' in the engineering application of functional material design for vehicles.

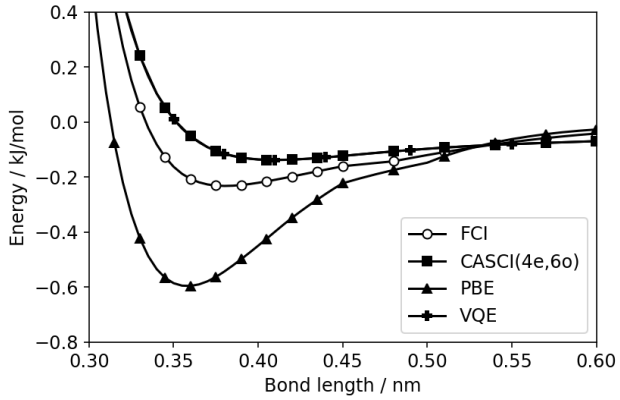


Fig.1 Comparison of H_2- H_2 dissociation energy profile for four representative electronic state theories

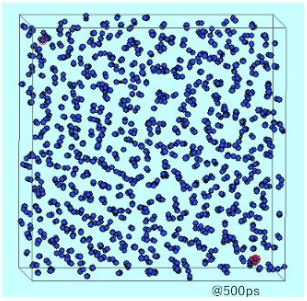
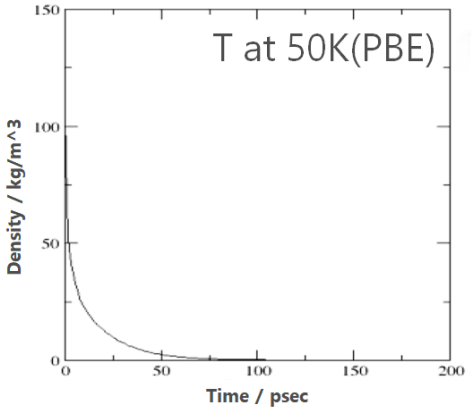


Fig.2 Applied periodic boundary structure in this study (500 psec in molecular dynamics)



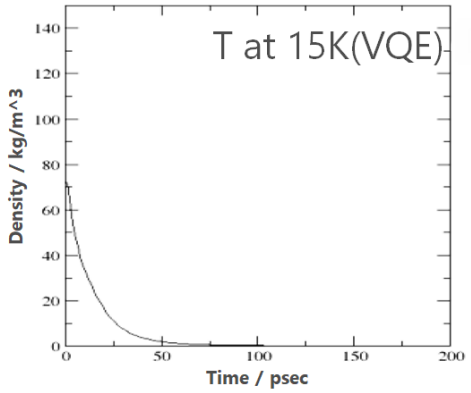


Fig.3 Comparison of hydrogen vaporization behavior with DFT(PBE) and VQE in molecular dynamics (Experimental vaporization temperature is 20K)