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Diffusion Monte Carlo method for evaluating Hamaker constants
RYO MAEZONO, KENTA HONGO, JAIST — We evaluated Hamaker's constants for Si_6H_{12} (CHS) to investigate its wettability, which is industrially useful but no references available. The constant is fundamental for wettability, but not directly accessible by experiments. Ab initio estimations are therefore in demand, and surely give an impact for broader fields such as tribology where the wettability plays an important role. The evaluation of binding curves itself could be a big challenge if it is applied to a practical molecule such as CHS, because highly accurate descriptions of electron correlations in vdW bindings get tough for such larger sizes with anisotropy. We applied DMC to overcome this difficulty, showing a new direction for wettability issues. Since ab intio estimations rely on simple assumptions such as additivity (and hence we denote it as A_{add}), it would include biases. Taking a benzene as a benchmark, we compared A_{add} evaluated from several available binding curves with other reported A_L (estimations based on Lifshitz theory). By the comparison, we get trends of biases in A_add due to non-additivity and anisotropy because A_L is expected to capture these effects to some extent in macroscopic manner. The expected trends here surprisingly well explain the series of results for CHS.

Ryo Maezono
JAIST

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