

Abstract Submitted
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Evaluation of Hamaker coefficients using Diffusion Monte Carlo method RYO MAEZONO, KENTA HONGO, School of Information Science, JAIST, Japan — We evaluated the Hamaker's constant for Cyclohexasilane to investigate its wettability, which is used as an ink of 'liquid silicon' in 'printed electronics'. Taking three representative geometries of the dimer coalescence (parallel, lined, and T-shaped), we evaluated these binding curves using diffusion Monte Carlo method. The parallel geometry gave the most long-ranged exponent, $\sim 1/r^6$, in its asymptotic behavior. Evaluated binding lengths are fairly consistent with the experimental density of the molecule. The fitting of the asymptotic curve gave an estimation of Hamaker's constant being around 100 [zJ]. We also performed a CCSD(T) evaluation and got almost similar result. To check its justification, we applied the same scheme to Benzene and compared the estimation with those by other established methods, Lifshitz theory and SAPT (Symmetry-adopted perturbation theory). The result by the fitting scheme turned to be twice larger than those by Lifshitz and SAPT, both of which coincide with each other. It is hence implied that the present evaluation for Cyclohexasilane would be overestimated.

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