E2-05 Development of a new functional form for the interaction energy of inert gases

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A potential energy functional form for the interaction of He atoms in gaseous phase was developed by using Hartree-Fock-Dispersion (HFD) potential function.

Potential energy of helium as a function of the interatomic distance, r, obtained from the HFD function was fitted to the proposed functional form, using linear-least-squared-fitting procedure. The HFD function consists of 9 parameters, while the proposed function contains only 4 parameters and the function itself is easy to handle by the computer in molecular dynamics and Monte Carlo simulations of helium in gaseous as well as condensed phases, which excessive force and energy calculations are needed.

The new potential function is compared graphically with HFD function and other available potential energy functions for He-He interaction. The virial coefficients of He gas at various temperatures were calculated using the proposed potential energy function and compared with those calculated from HFD. An excellent agreement between HFD results and ours is observed. The advantage of this simple functional form in computer simulations is discussed.

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