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Combination Rule for Homonuclear Dipole Dispersion Coefficients

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Abstract : In the ambit of intermolecular interactions, a combination rule is defined as a relation linking a potential parameter for the interaction of two unlike species with the same parameters for interaction pairs of like species. Some of their most exemplificative applications cover the construction of molecular dynamics force fields and dispersion-corrected density functionals. Here, an extended combination rule is proposed, relating the dipole-dipole dispersion coefficients for the interaction of like target species to the same coefficients for the interaction of the target and a set of partner species. The rule can be devised in two different ways, either by uniform discretization of the Casimir-Polder integral on a Gauss-Legendre quadrature or by relating the dynamic polarizabilities of the target and the partner species. Both methods return the same system of linear equations, which requires the knowledge of the dispersion coefficients for interaction between the partner species to be solved. The test examples show a high accuracy for dispersion coefficients (better than 1% in the pristine test for the interaction of Yb atom with rare gases and alkaline-earth metal atoms). In contrast, the rule does not ensure correct monotonic behavior of the dynamic polarizability of the target species. Acknowledgment: The work is supported by Russian Science Foundation grant # 17-13-01466.

Keywords : combination rule, dipole-dipole dispersion coefficient, Casimir-Polder integral, Gauss-Legendre quadrature
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