Abstract Submitted
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An Efficient Coupled Dipole Method: TCDM[1] HYE-YOUNG KIM, Southeastern Louisiana Univ — An overview of a memory-efficient and cost-effective method, called Trace-Coupled Dipole Method (TCDM), which can accurately predict the van der Waals (VDW) forces between dielectric materials will be presented. CDM is an intrinsically atomistic method which includes all the many-body interaction terms self-consistently. TCDM, an alternative way to execute CDM, is to obtain VDW interaction energy by calculating the trace of a 3NX3N matrix, rather than its eigenvalues. It will be demonstrated that the power series expansion in TCDM is equivalent to that of the perturbation theory. The advantage of adopting TCDM over the conventional perturbation theory or CDM will also be discussed. The use of TCDM will make it practical for any interested future users to calculate the accurate VDW interaction in large systems like those found in computer simulation studies without serious increase in computational burden.

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