Recent advances in first-principles force field development using SAPT: Approaching quantitative accuracy with transferable site-site potentials

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Recent advances in first-principles force field generation utilizing symmetry adapted perturbation theory (SAPT) will be described. Our prior work has established that utilizing the SAPT energy decomposition and fitting atomic force field parameters on a term-by-term basis enables the generation of accurate force fields that exhibit high transferability between physical (temperature, pressure…) and chemical environments. During the discussion, an emphasis will be placed on several recent developments that enable significant increases in the fidelity of the fitted force field to the underlying SAPT data, without significantly increasing computational cost or sacrificing transferability. These include: derivation and application of a novel short-range functional form to model exchange repulsion and charge penetration; utilization of iterated stockholder atoms (ISA) partitioning to derive selected force field parameters from first principles; and straightforward incorporation of "short range" atomic anisotropy where essential (e.g. for atoms with "lone pairs").