Grimme の分散力補正 DFT 法で計算したヘテロ原子の分散力の精度

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Accuracy of intermolecular interaction energies of molecules including hetero atoms using Grimme's dispersion corrections

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Intermolecular interaction potentials for 11 complexes were calculated using several functionals with Grimme's dispersion correction methods of the D2, D3 and D3BJ versions. The calculated potentials were compared with the CCSD(T) level potentials to evaluate the accuracy of the dispersion corrected DFT methods for calculating the intermolecular interaction energies. The performance of the calculations depends strongly on the choice of functional and dispersion correction method. Neither combination of the functionals and the dispersion correction methods can reproduce well the CCSD(T) level interaction potentials of all the 11 complexes. The improvement of the functionals from GGA to hybrid GGA or meta GGA is not essential for improving the performance. The interaction potentials for the benzene and CF_4 dimers calculated by the dispersion corrected DFT methods are shown in Figure. The dispersion-corrected DFT potentials for hydrocarbons often well reproduce CCSD(T) calculations well, while those for molecules including heteroatoms often do not match well.

Keywords : Intermolecular interaction, Dispersion correction, DFT calculation, Hetero atom, Accuracy of calculation

種々の汎関数と Grimme の D2, D3, D3BJ 分散力補正法を使い 11 種の会合体の分子間相互作用ポテンシャルを計算し、計算精度を検討するために CCSD(T) 法で計算した相互作用ポテンシャルと比較した。計算精度は汎関数と分散力補正法の選択に強く依存した。どの汎関数と分散力補正を組み合わせても 11 種の会合体全ての CCSD(T) 法での相互作用ポテンシャルを良く再現することはできなかった。また、汎関数を GGA から hybrid GGA やメタ GGA に改良しても必ずしも CCSD(T) 計算との一致は改善しなかった。図のベンゼンのように炭化水素では多くの組み合わせが CCSD(T) 計算をよく再現したが、ヘテロ原子が入った CF_4 等の分子では再現の困難な場合がある。