Abstract Title:

Extending density functional calculations beyond pure water

Author:

Eunji Sim, Department of Chemistry, Yonsei University, 50 Yonsei-ro Seodaemun-gu, Seoul 03722, Korea

Abstract:

Density-corrected density functional theory (DC-DFT) reduces density-driven energy errors caused by errors in self-consistent densities by using a more accurate density instead.[1] This presentation reviews recent progress in functional design and applications based on DC-DFT, including functional error analysis utilizing density insensitive systems.[2] In particular, the systematic application of the DC-DFT principles combined with dispersion correction was used to design the HF-r^{2}SCAN-DC4 functional, which excellently captures interactions between water molecules as well as important noncovalent interactions between water and bio- and organic molecules.[3]

[1] M.-C. Kim, E. Sim, and K. Burke "Understanding and Reducing Errors in Density Functional Calculations", Phys. Rev. Lett. 111, 073003 (2013)
[2] E. Sim, S. Song, S. Vuckovic, and K. Burke, "Improving Results by Improving Densities: Density-Corrected Density Functional Theory," J. Am. Chem. Soc., 144, 6625 (2022).
[3] S. Song, S. Vuckovic, Y. Kim, E. Sim, and K. Burke, "Extending density functional theory with near chemical accuracy beyond pure water," (submitted, 2022).