**Abnormalities in Density Functional Calculations
 on Ions and Radicals and its solution:
 Density-Corrected Density Functional Theory**

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In this presentation, we introduce a systematic and practical way to correct various abnormalities in density functional theory(DFT) using density-corrected DFT (DC-DFT)[1-5]. DFT is a widely used electronic structure calculation method due to its good balance between accuracy and computational cost. One of the challenges in DFT is calculating equilibrium structures, electronic structures, and potential energy surfaces of anions and radicals, where it suffers greatly from the self-interaction error. This includes unphysical positive HOMO energies for anions, predicting incorrect ground state geometry for radical complexes, incorrect dissociative behavior for molecular species.

Here, we perform a very simple analysis on the source of error of DFT calculations and classify DFT calculations into two different groups: normal and abnormal calculation. We show that one can easily determine an abnormal calculation, and “cure” it using DC-DFT. We apply DC-DFT on problematic cases especially for ions and radicals and show it gives excellent results.

1. M.-C. Kim, E. Sim, and K. Burke, J. Chem. Phys. 134(17), 171103 (2011)
2. M.-C. Kim, E. Sim, and K. Burke, Phys. Rev. Lett., 111, 073003 (2013)
3. M.-C. Kim, E. Sim, and K. Burke J. Chem. Phys. 140, 18A528 (2014)
4. M.-C. Kim, H. Park, S. Son, E. Sim, and K. Burke, J. Phys. Chem. Lett. 6, 3802-3807 (2015)
5. A. Wasserman, J. Nafziger, K. Jiang, M.-C. Kim, E. Sim, and K. Burke, Ann. Rev. Phys. Chem., 68, 555-581 (2017)