An efficient *ab initio* computational method for extended Hubbard interactions

Young-Woo Son

Korea Institute for Advanced Study, Seoul 02455, Korea

In this talk, I will present my group and coworkers' recent efforts to develop an efficient first-principles calculation method to compute electronic structures, phonon dispersions, and electron-phonon interactions of correlated materials [1-6]. The method can obtain self-consistent on-site and inter-site Hubbard interactions using newly developed position-dependent pseudohybrid functionals [1]. All the interactions can be evaluated within self-consistent loops without serious additional costs such that the method can be as fast as conventional *ab initio* methods with (semi)local density approximations while its accuracy is comparable to sophisticated methods such as *GW* approximation [1,3,5,7]. I will demonstrate that the newly developed method can compute accurate quasiparticle bands structures of various correlated materials [1-4], phonon dispersions of correlated insulators [5] as well as charge-ordered materials [6]. Considering its improved accuracy with low computational costs, our new computational method is expected to contribute massive database-drivien high-troughput quantum materials researches.

[1] S.-H. Lee and Y.-W. Son, arXiv:1911.05967
[2] J. Huang *et al.*, arXiv:2008.02417
[3] W. Yang *et al.*, arXiv:2106.07201
[4] Y.-W. Son *et al.*, arXiv:2201.09456
[5] W. Yang *et al.*, arXiv:2205.02972
[6] B. G. Jang *et al.*, arXiv:2205.02470
[7] M. Kim et al., in preparation.