Title of Talk: Illustration of Chemical Bonding and Its Guidance to Rational Materials Design

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Abstract:
For newly developed chemical systems, the investigation of its underlying chemical bonding mechanism is particularly important. However, the use of classical chemical concepts on novel systems is surprisingly rare. One of the reasons might be the limited availability of chemical analysis methods for condensed phase calculations, especially for those using plane-wave basis sets. For condensed phase systems, several analysis methods can be utilized, such as electron localization function, partial density of states and charge density difference plots. Recently, charge topology analysis according to Bader’s scheme has been made feasible by Henkelman et al. In this talk, another implementation for characterizing the bond critical point will be described. Such an implementation allows us to analyze three dimensional charge density grids which can be generated by Gaussian package and VASP. By using this implementation, we have successfully explored the role of electrostatic effect on engineering reaction barriers for: 1) oxygen reduction reaction (ORR) on noble metals; and 2) CO activation process on cobalt surfaces.