Nuclear Orbital plus Molecular Orbital (NOMO) Theory: Overview and Recent Progress

Résumé

The author's group first proposed the simultaneous determination method for both nuclear and electronic wavefunctions in 1998 [1]. The theory was reformulated for applying to general systems as the nuclear orbital plus molecular orbtial (NOMO) theory [2]. The accuracy of the NOMO theory was improved from the two viewpoints: namely, many-body effect such as nucleus-electron (n-e), nucleus-nucleus (n-n), and electron-electron(e-e) correlations [3-6] and treatments of nuclear motions such as translations and rotations in addition to vibrations [7-9]. Similar approaches have been examined by several research groups [10-14]. (For more details, please see reviews [15-18].)
The applications of the NOMO and/or related theories have covered the wide area: for example, (1) vibrational excitations [19], (2) isotope effects on geometries [20-22], kinetics [23,24], and weak interactions [25,26], (3) proton tunnelings [27], and (4) positron affinities and positron annihilation rates [28-32].

Reyes and coworkers combined the propagator method with the NOMO (or APMO, anyparticle MO) method in order to evaluate proton affinities [33,34]. Reyes's group and the author's group collaborated to further extend the linear-scaling divide-and-conquer method [35-37] for the second-order proton propagator method, as denoted by NOMO/DC-PP2 [38].

In this presentation, the theoretical background of NOMO will be first overviewed and recent progress of NOMO will be intensively explained.

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