First principles calculation of exotic particle systems

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Interactions of exotic particles, including positron, antiproton, and nuclear isotopes, with electrons, atoms, and molecules, have drawn significant attension due to their intriguing properties and wide-range potential applications in scientific and technological fields. One of the most notable is the positron (e^+), the antimatter counterpart of the electron. Positron and positronium (hydrogen-like bound state between a poistron and an electron, Ps) have been used as versatile diagnostic tools in many areas, including materials science and medicine. In bulk materials, positrons are trapped by open-volume defects and annihilate with electrons, emitting gamma rays. This process enables the non-invasive characterization of materials. Similar characterizations may be possible for finite-size multi-atomic systems.

We will present recent progress in first-principles studies for various positron complexes; few-body or fewer multi-atoms[1-2], molecules[3], and clusters[4]. For small systems, we have applied the explicitly-correlated, quantum Monte Carlo, and the multi-component molecular orbital calculations. The positron can form electronically stable bound state intermediating repulsive two anions, akin to the single electronic chemical bond, which was indentified as convalent positron bond[5]. There are complicated and multifaceted compositions of the Ps-atom or Ps-molecule bound states due to different stabilization mechanisms arising from electon-positron correlation[1-2]. For larger systems such as biomolecules, microsolvents, aqueous complexes, etc., positrons also exhibit various binding and annihilation properties that depend on physical and chemical characteristics inherent to the host molecules, including electrostatic properties and conformational structures[3,4]. We have also developed the density functional approach employing the electron-positron correlation-polarization potential, aming at studying larger molecular aggregates. We performed a case study for positron bindingin water microsolvent cluseters, and revealed internally- and surface-bound positron states influenced by conformational structures, resembling the bound excess electrons in water anions or positrons trapped in vacancies of bulk systems. We will present the fascinating aspects of the positron, which exhibits flexibility comparable to the electron, in relation to the characteristics of materials, guided by the first-princples.

References

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