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Quantum Computational Chemistry in Perovskite Nanomaterials

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Abstract

In quantum computational chemistry, molecular orbital (MO) method is widely utilized for calculating molecular system. On the other hand, in solid state chemistry, band theory is often utilized for solid system, where periodic boundary condition can be applied. In our previous research, we have explored MO approach for calculating solid system, especially perovskite nanomaterial. It is because our constructed "Chemical bonding rule" enables us to characterise chemical bonding property between atoms.

Chemical bonding rule
For molecular orbitals including outer shell electrons, check whether orbital overlap exists or not
-With orbital overlap: Covalent
-Without orbital overlap: Ionic

After introducing our MO approach, we will show our previous calculation results of ion conducting perovskites:
(1) Lithium ion conductor for lithium ion battery
(2) Oxide ion and proton conductors for solid oxide fuel cell (SOFC)

References

[1]T. Onishi, *Quantum Computational Chemistry-Modelling and Calculation for Functional Materials* (Springer Nature), 1-290, 2018
[2]T. Onishi, *Adv. Quant. Chem.* 70, 31-67, 2015
[3]T. Onishi, *Adv. Quant. Chem.* 64, 31-81, 2012