Curriculum Vitae

Rundong Zhao

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Employment:

02/2018-present	Postdoctoral Associate, Duke University, with Prof. Volker Blum.
08/2016-02/2018	Postdoctoral Research Fellow, Hong Kong Baptist University, with Prof. Michel. A. Van Hove.
11/2015-08/2016	Visiting Scholar, Beijing Computational Science Research Center.

Education:

2010-2015	Ph.D, College of Chemistry and Molecular Engineering, Peking University, with Prof. Wenjian Liu.
2006-2010	B.S., School of Physics, Shandong University.

Research interests:

1. Relativistic electronic structure theory in periodic systems.

   The main task of my PhD thesis was to develop methods and codes in the areas of quantum chemistry and solid state physics: the program I developed – as a branch of Beijing Density Functional (*BDF*) package – is a first-principles DFT code for ground state electronic structure calculations on periodic systems. Based on this code, the exact two-component (X2C) relativistic method was further implemented, with X2C currently being the most efficient method (based on, but beyond the Dirac equation) that can deal with full relativistic effects (including both scalar relativistic effects and spin orbit coupling (SOC) effect) in electronic structures. In the AIMS group at Duke, I am now trying to improve the accuracy of the SOC corrections in *FHI-aims* package which adopts numeric atomic-centered orbitals (NAOs), and to embed X2C in it.

2. Intermolecular interactions.

   During the visiting time at Beijing Computational Science Research Center (CSRC), my interest was focused on the application research in intermolecular interaction in chemical systems: we explored specifically the intermolecular orbital interaction between monomers and thus proposed a new model (beyond the classical electrostatic model) to describe π-involved interactions, i.e. π-π stacking and aqueous-π interactions.

3. Molecular machines, especially molecular rotors and gears. The project of my postdoctoral research in Prof. Michel Van Hove's group was to design (and to reveal the deep theoretical mechanism of) rotational molecules that are expected to transmit energies and rotational motion in the form of interlocking gears on surfaces (metal/graphene). We successfully designed several prototypes of molecular gears, from triple-arm gears (PF_3 or NH_3 molecules attached to Cu surfaces) to multi-arm

gears (a 5-membered carbon ring substituted with 5 -CN groups or a 6-membered carbon ring substituted with 6 -C≡CH groups attached to graphene sheets), that can be aligned on surfaces and transmit rotational motion from its source to a point of application, as in macroscopic machines.

4. I am also interested in the electron tunneling effect which gains lots of attention in attosecond science and semiconductor industry in recent years. We have developed a new algorithm named projected Green's function (PGF) method to calculate the tunneling lifetime of an electron escaping from an atom or from quantum wells.

Publications:

1. Rundong Zhao, Fei Qi, Rui-Qin Zhang, Michel A. Van Hove. "How Does the Flexibility of Molecules Affect the Performance of Molecular Rotors?" *J. Phys. Chem. C*, DOI: 10.1021/acs.jpcc.8b08158 (2018).
2. Yan-Ling Zhao, Rundong Zhao, Fei Qi, Rui-Qin Zhang, Michel A Van Hove. "Substrate-mediated and temperature-modulated long-range interactions between bromine adatom stripes on Cu (111)". *Appl. Surf. Sci.*, 463, 253-260 (2018).
3. Faiz Ur Rahman, Rundong Zhao, Yanoar Pribadi Sarwono, Rui-Qin Zhang. "A scheme of numerical solution for three-dimensional isoelectronic series of hydrogen atom using one-dimensional basis functions". *Int. J. Quantum Chem.*, e25694 (2018).
4. Klaus E. Hermann, Fei Qi, Rundong Zhao, Rui-Qin Zhang, Michel A. Van Hove. "Fragment Motion in Motor Molecules: Basic Concepts and Application to Intra-Molecular Rotations". *Phys. Chem. Chem. Phys.*, 20(33), 21487-21497 (2018).
5. Rundong Zhao, Fei Qi, Yan-Ling Zhao, Klaus E. Hermann, Rui-Qin Zhang, Michel A. Van Hove. "Interlocking Molecular Gear Chains Built on Surfaces". *J. Phys. Chem. Lett.*, 9(10), 2611 (2018).
6. Rundong Zhao, Yan-Ling Zhao, Fei Qi, Klaus E. Hermann, Rui-Qin Zhang, Michel A. Van Hove. "Interlocking Mechanism Between Molecular Gears Attached to Surfaces". *ACS Nano*, 12(3), 3020 (2018).
7. Chak-Shing Kwan, Rundong Zhao, Michel A. Van Hove, Zongwei Cai, Ken Cham-Fai Leung. "Higher-generation type III-B rotaxane dendrimers with controlling particle size in three-dimensional molecular switching". *Nat. Comm.*, 9, 497 (2018).
8. Rundong Zhao, Rui-Qin Zhang. "Intermolecular orbital interactions in π systems". *Mol. Phys.*, 116 (7-8), 978 (2018).
9. Hong-Shuai Tao, Rundong Zhao, Yanoar Pribadi Sarwono, Rui-Qin Zhang. "Improved projected Green's function approach to electron tunneling lifetime calculations in quantum wells". *Phys. Rev. B.*, 96, 235428 (2017).
10. Rundong Zhao, Yanoar Pribadi Sarwono, Rui-Qin Zhang. "Tunneling lifetimes of electrons escaping from atoms under a static electric field". *J. Chem. Phys.*, 147, 064109 (2017).
11. Rundong Zhao, Rui-Qin Zhang. "Beyond the electrostatic model: the significant roles of orbital interaction and dispersion effects in aqueous-π systems". *Phys. Chem. Chem. Phys.*, 19, 1298 (2017).
12. Rundong Zhao, Rui-Qin Zhang. "A new insight into π−π stacking involving remarkable orbital interactions". *Phys. Chem. Chem. Phys.*, 18, 25452 (2016).

13. Rundong Zhao, Yong Zhang, Yunlong, Xiao, Wenjian Liu. "Exact two-component relativistic energy band theory and application". *J. Chem. Phys.*, 144, 044105 (2016).

Talks:

1. "Relativistic energy band theory: the exact two-component algorithm and its code implementation". Invited Talk in CSRC Seminars, August 07, 2018. Beijing Computational Science Research Center (CSRC), Beijing.
2. "Interlocking mechanism between molecular gears attached to surfaces". The 20th PSHK (Physical Society of Hong Kong) Conference, June 16–17, 2017. Hong Kong University of Science and Technology, Hong Kong.
3. "Electron tunneling time in atomic systems: a projected Green's function approach". The 9th Joint Meeting of Chinese Physicists Worldwide, July 17–20, 2017. Tsinghua University, Beijing.
4. "Interlocking mechanism between molecular gears attached to surfaces". International Symposium on Nanomachines: Powering Molecules. November 29 – December 1, 2017. Hong Kong Baptist University, Hong Kong.

Appendix: a brief introduction of the X2C-BAND code.

X2C-BAND is an extended branch of the Beijing Density Functional (*BDF*) code − a program package with relativistic calculation capability for molecular systems, developed several years ago by professor Wenjian Liu's group at Peking University. The *X2C-BAND* was mainly designed to perform nonrelativistic, scalar relativistic and fully-relativistic ground state electronic structure calculations for 1D, 2D and 3D periodic systems, including insulators, semiconductors and metals.

As the author of *X2C-BAND*, I at first developed it for nonrelativistic cases, following the framework of *FHI-aims*, *ADF-BAND* and *Quantum-ESPRESSO* packages; and the relativistic effects can be in principle treated by employing the Dirac equation. Instead of directly using Dirac equation which contains four components thus involving large computational demand in applications, we proposed the X2C method which adopts a two-component algorithm (the dimension of the Hamiltonian matrix is half of that in traditional four-component methods) but without loss of accuracy. In a word, the X2C method holds both the efficiency of two-component methods and the accuracy of four-component methods.

Below is the main description of this code:

1. It is an all-electron full-potential program based on linear combination of atomic orbitals (LCAO) and Density Functional Theory (DFT).
2. Matrix elements are evaluated using numerical integrations on atom-centered grids with Becke partition, with the radial grids generated by the Chebyshev-Gauss scheme and the angular grids generated by the Lebedev quadrature scheme.
3. Coulomb potential is obtained through the multipolar expansion method, in which the Ewald technique should be adopted to treat long range terms.
4. For Brillouin Zone sampling, we use the special K points scheme and apply point group symmetry to reduce the symmetry-related points.

5. The LDA (VWN) and GGA (PBE and PBEsol) exchange-correlation functionals are implemented as a pilot start.
6. The SCF procedure starts from a model density and a model potential interpolated using the electron densities of free atoms (the free atoms are solved in advance, before starting the SCF iteration of a molecule or solid). As the initial Hamiltonian matrix and overlap matrix have been generated, the code can solve Kohn-Sham equation for nonrelativistic cases, or solve Dirac-Kohn-Sham equation (or preferably X2C equation) for relativistic cases. Acceleration algorithms, e.g. DIIS, for SCF are adopted.
7. Band structures, DOS and partial DOS can be drawn automatically. Cell energy can be obtained (using the general transition state method) for geometry optimizations. The functionality of calculating Z_2 topological invariant for 2D and 3D topological insulators is also available.