

## ABSTRACT

Motivated by the recently renewed interest in the High T<sub>c</sub> superconducting bismuth perovskites, we investigate the electronic structure of the parent compounds ABiO<sub>3</sub> (A = Sr, Ba) using ab initio methods and tight-binding modeling. We use the density functional theory in the local density approximation to understand the role of various contributions in shaping the ABiO<sub>3</sub> band structure near the Fermi level. It is established that hybridization involving Bi-6s and O-2p orbitals plays the most important role. The opening of a gap with the onset of the breathing distortion is shown to be associated with condensation of holes onto a 1g-symmetric molecular orbitals formed by the O-2p $\sigma$  orbitals on the collapsed BiO<sub>6</sub> octahedra. The primary importance of oxygen p states is thus revealed, in contrast to a popular picture of a purely ionic Bi<sup>3+</sup>/Bi<sup>5+</sup> charge-disproportionation. A single band model involving an extended molecular orbital of both Bi-6s and a linear combination of six O-2p orbitals is derived which provides a very good description of the low energy scale bands straddling the chemical potential.

In addition, a parameter based phase diagram associated with materials incorporating “skipped valence” ions is developed. A crossover from a bond disproportionated (BD) to a charge-disproportionated (CD) system in addition to the presence of a new metallic phase is observed. We argue that three parameters determine the underlying physics of the BD-CD crossover when electron correlation effects are small: the hybridization between O-2p $\sigma$  and s orbitals of the B cation in ABO<sub>3</sub>, their charge-transfer energy ( $\Delta$ ), and the width of the oxygen sub-lattice band ( $W$ ). In the BD system, we estimate an effective attractive interaction  $U$  between holes on the same O-a1g molecular orbital. Later, we show the possibility of surface electron doping of the bismuthates via adatom and finally, we propose a new class of materials, namely heterostructure composed of LaLuO<sub>3</sub>(LLO) and SrBiO<sub>3</sub>(SBO), that can host coexisting electron and hole gases and potentially high temperature superconductivity at their two opposite interfaces. We argue that electronic reconstruction is the dominant mechanism for solving the diverging potential (“polar catastrophe”) in this system which in return results in simultaneous electron and hole doping of LLO/SBO/LLO heterostructure at its interfaces. The electronic structure of this system suggests the electron-hole gas interactions can be tuned with the potential of obtaining excitonic insulating phases.

## BIOGRAPHICAL NOTES

Academic Studies: B.Sc. University of Toronto, 2010  
M.Sc. University of British Columbia, 2013

## GRADUATE STUDIES

Field of Study: Theoretical Condensed Matter physics

### Courses

		Instructors
PHYS 500	Quantum Mechanics I	Dr. R. Raussendorf
PHYS 501	Quantum Mechanics II	Dr. I. Affleck
PHYS 502	Condensed Matter Physics I	Dr. M. Franz
PHYS 504	Special Relativity and Classical EM	Dr. D. Louis-Martinez
PHYS 508	Quantum Field Theory II	Dr. A. Zhitnitsky
PHYS 509C	Theory of Measurements	Dr. S. Oser
PHYS 516	Statistical Mechanics	Dr. F. Zhou
PHYS 521D	Group Theory Methods in QM	Dr. G. Semenoff
PHYS 526	Quantum Field Theory I	Dr. M. Van Raamsdonk
PHYS 855	Computational methods for Quantum Materials	University of Sherbrooke

### AWARDS

The Faculty of Science Ph.D. Tuition Award

### SELECTED PUBLICATIONS

- "Hybridization effects and bond disproportionation in the bismuth perovskites", Kateryna Foyevtsova, Arash Khazraie, Ilya Elfimov, and George A. Sawatzky Phys. Rev. B 91, 121114(R) (2015)
- "Oxygen holes and hybridization in the bismuthates" Arash Khazraie, Kateryna Foyevtsova, Ilya Elfimov, and George A. Sawatzky Phys. Rev. B 97, 075103 (2018)
- "Bond versus charge disproportionation in the bismuth perovskites" Arash Khazraie, Kateryna Foyevtsova, Ilya Elfimov, and George A. Sawatzky Phys. Rev. B 98, 205104 (2018)
- "Electron and hole 2D gasses at interfaces of SrBiO<sub>3</sub>/LaLuO<sub>3</sub> heterostructures", Arash Khazraie, Ilya Elfimov, Kateryna Foyevtsova, and George A. Sawatzky. under preparation

### SELECTED PRESENTATIONS

Cutting-Edge Topics in Quantum Materials (ParisEdge2017), Paris, France, 2017

### SUPERVISORY COMMITTEE

Dr. George Sawatzky, (Research Supervisor), Dr. Ilya Elfimov, (Research Supervisor)  
Dr. Joerg Rottler  
Dr. Jeremy Heyl  
Dr. Doug Bonn



a place of mind

THE UNIVERSITY OF BRITISH COLUMBIA

## Graduate and Postdoctoral Studies

### PROGRAMME

The Final Oral Examination  
For the Degree of

DOCTOR OF PHILOSOPHY  
(Physics and Astronomy)

### ARASH KHAZRAIE ZAMANPOUR

B.Sc., University of Toronto, 2010

M.Sc., University of British Columbia, 2013

Friday, December 14, 2018, at 2:00 pm

Room 311, Brimacombe Building, 2355 East Mall.

*Latecomers will not be admitted*

**"A first principle study of the electronic structure of the bismuthates"**

### EXAMINING COMMITTEE

Chair:

Dr. Elod Gyenge (Chemical and Biological Engineering)

Supervisory Committee:

Dr. George Sawatzky, (Research Supervisor)

Dr. Joerg Rottler

Dr. Jeremy Heyl

University Examiners:

Dr. Roman Krems (Chemistry)

Dr. Philip C E Stamp (Physics and Astronomy)

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