Report on Workshop "Topological Insulators and Non-Perturbative Spin-Orbit Coupling"

CECAM-HQ-EPFL, Lausanne, Switzerland

January 9–11, 2012

CECAM, Psi-k, ESF

Oleg Yazyev (EPFL),
Joel Moore (UC Berkeley),
David Vanderbilt (Rutgers U)

http://www.cecam.org/workshop-564.html

REPORT

Scope of the workshop.– Topological insulators are the recently discovered materials that have a bulk electronic band gap, but also exhibit conducting surface states. These surface states, originating from the combination of strong spin-orbit interactions and time-reversal symmetry, exhibit a number of novel properties such as the chiral spin textures and topological protection from backscattering. Many materials have now joined the list of confirmed topological insulators. Related materials include quantum anomalous Hall insulators, topological superconductors, and Weyl semimentals.

The emerging field of topological insulators and related materials has now become one of the most rapidly developing areas of physics. This workshop is the first attempt to bring together active computational electronic structure researchers pioneering the field of topological insulators. The topics addressed by the speakers included methodological developments, first-principles investigation of novel physical properties of known topological insulators, and in silico discovery of new topological materials. In addition, several leading phenomenological theorists and experimentalists participated in the workshop.

General aspects and methodology.– The introductory talk given by Joel Moore (Berkeley) covered the theoretical basics of the field and highlighted a number of problems which can be solved by the computational physics community. David Vanderbilt (Rutgers) and Ivo Souza (San Sebastian) discussed the calculations of orbital magnetoelectric response. Raffaele Resta (Trieste) presented a local Chern number approach towards mapping topological order in real space. On the purely methodological side of the field, Andrea Dal Corso presented his new PAW methodology which naturally includes spin-orbit interactions. Hubert

Ebert (Munich) addressed the problem of modeling ARPES spectra using the so-called one-step-model of photoemission that describes excitation, transport to the surface and the escape to the vacuum in a coherent way. The problem of modeling electronic transport properties of topological insulators was addressed by Stephan Roche (Barcelona). Finally, the entertaining talk of Pekka Pyykkö (Helsinki) covering the role of spin-orbit interactions in heavy-element chemistry earned special attention.

Experiments.– The first session of the workshop included two experimental presentations. The first talk was given by Zahid Hasan (Princeton) who pioneered the field of 3D topological insulators. Hasan spoke both about the discovery of bulk topological insulators as well as about recent works on the Tl–Bi–S–Se system in which the topological phase transition can be achieved by tuning the chemical composition. This system was proposed as a platform for studying Weyl fermion physics. He also covered their studies of magnetically doped bismuth chalcogenide topological insulators. The second experimental talk was given by Marco Grioni (EPFL) who presented ARPES investigations of surface systems with strong spin-orbit interactions.

Bismuth chalcogenide topological insulators.– Bismuth chalcogenides (Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3) are currently the most extensively investigated bulk topological insulators, both experimentally and theoretically. Several speakers focused specifically on these materials. Oleg Yazyev (EPFL) reported calculations of spin polarization of topologically protected charge carriers in these materials and proposed a spintronic device based on thin films of these materials capable of independent control of spin and charge transport. He also covered the recent advances in *GW* quasiparticle band structure calculations of these materials. Hyoung Joon Choi (Yonsei) reported calculations of the orbital angular momentum of the surface states and an investigation of the topologically protected states at the side surfaces of these materials. Jürgen Henk (Halle) presented the results of their calculation on Mn-doped Bi_2Te_3. Kyungwha Park (Virginia Tech) reported the results of first-principles calculations on interfaces between bismuth chalcogenides and silicon.

Novel topological insulators.– Predicting novel topological insulators *in silico* is currently the major direction of computational first-principles research in this field. Arun Bansil (Boston) and Binghai Yan (Bremen) covered their theoretical prediction of thallium-based topological insulators derived from bismuth chalcogenides, which was followed by experimental confirmation. Eugene Chulkov (San Sebastian) introduced a large family of bismuth-based topological insulators that contain group-IV elements. Stanislav Chadov (Mainz) presented an extensive search for topological insulators in the family of half-Heusler alloys. Many speakers presented even more dramatic departures from known topological insulators. For instance, Hai-Jun Zhang (Stanford) considered strongly correlated actinides while Zhong Fang (Beijing) spoke about Ag_2Te and $HgCr_2Se_4$.

Topological electronic phases in graphene.– An important part of the workshop concerned the 2D topological electronic phases on the honeycomb lattice. Motivated by the models introduced by Haldane and by Kane and Mele, a number of research groups aim at realizing these phases in practice. Jaroslav

Fabian (Regensburg) presented their results on the origin of intrinsic spin-orbit gap in graphene and proposed a recipe towards enhancing spin-orbit coupling in graphene by means of hydrogen adatoms. Joaquin Fernandez-Rossier (IINL-Braga) considered the Kane-Mele model in the presence of electron-electron interaction introduced via the Hubbard term. Stefan Blügel (Jülich) discussed the possibility of realizing the quantum anomalous Hall effect by depositing heavy-element magnetic adatoms on graphene.

Report on selected discussion.– Several speakers identified important issues that have to be addressed by the computational community. In particular, in his introductory talk Joel Moore (Berkeley) highlighted the problem of interfaces between topological insulators and other materials that can be addressed by means of first-principles computations. In particular, he mentioned the interfaces with magnetic materials and superconductors, which are important in the context of realizing Majorana fermion systems. A somewhat related aspect concerns the modeling of thermoelectric properties of topological insulators and their interfaces. The last very important problem mentioned in this talk points at the need to develop an approach for defining the relevant topological invariants in strongly correlated systems. Many participants have also stressed the need in accurate beyond-DFT methodologies adapted to the topological electronic phases. Precise treatment of band gaps and relative band alignments, the properties poorly reproduced by the standard DFT schemes, are critical for modeling the topologically non-trivial properties of these materials. Oleg Yazyev (EPFL) presented the results of GW calculations of bismuth chalcogenide topological insulators, which essentially bridge the known disagreements between experimental data and DFT calculations for these materials. However, developing a consistent methodology involving both spin-orbit interactions and quasiparticle self-energy corrections remains a challenge. Hyoung Joon Choi (Yonsei) has mentioned the need to develop an approach for calculating orbital moments of electronic states in topological materials.

The workshop has certainly attained its two most important objectives identified in the proposal. First, the workshop allowed active researchers who have started working in this rapidly developing field to report their recent works. Second, the workshop allowed for unimpeded interaction between the representatives of the computational physics community on one side and several leading experimentalists and phenomenological theorists on the other. The joint efforts allowed determining a number of important objectives for future research. It is worth mentioning that despite the apparent diversity of the topological insulators community (which is typically the case for any emerging field), all participants of our workshop freely communicated to each other. One of the objectives of our workshop was to develop a strategy for the computational search for new topological insulators. Although several talks dedicated to the search for novel materials were given during the workshop, the speakers reported using different approaches such as the high-throughput investigation of a large number of structurally related compounds or the compositional changes of known topological insulators. It is now clear that only having several different approaches rather than one unified strategy can ensure rapid progress in

this direction. Another objective was related to the comparison of accuracy of various schemes for treating spin-orbit interactions in first-principles methodologies. The computations presented by the participants were making use of different DFT codes, which utilize different methods for calculating spin-orbit couplings. It turned out, however, that these methods tend to give very similar results. The main limitation in the predictive power of first-principles computations applied to topological insulators is thus density functional theory itself. Most of the participants have touched to some extent on the problem of determining topological phases from electronic structure calculations, which is the last objective of the workshop. A significant amount of progress is being made in this direction, but any conclusion would be preliminary at this point.

The topic of topological electronic phases enabled by spin-orbit interactions will certainly see a number of computationally-oriented workshops and conferences in the near future. A specialized workshop on this topic is already scheduled to take place in Bremen (August 13–17, 2012). We recommend that a follow-up CECAM workshop with a scope similar to ours should be held again within two years. For any such workshop, we recommend that it is absolutely necessary to actively involve experimentalists and phenomenological theorists in such computational events. This often-overlooked condition is crucial for the development of any emerging field, including that of topological insulators.

WORKSHOP PROGRAMME

Day 1 - January 9, 2012

8:45 to 9:00 – Welcome

9:00 to 9:40 – Joel Moore
Topological Insulators: Overview and Need for Electronic Structure Theory

9:40 to 10:20 – Zahid Hasan
Surface States in Topological Insulators and Superconductors: Discovery and Recent Results

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – Marco Grioni
Spin-Split States at Surfaces: the ARPES View

11:30 to 12:10 – Andrea Dal Corso
Projector Augmented-Wave Method with Spin-Orbit Coupling

12:10 to 12:30 – Hyungjun Lee
The Role of d-orbitals in the Spin-Orbit Induced Splitting in Noble Metal Surfaces

12:30 to 14:00 – Lunch

14:00 to 14:40 – Oleg Yazyev
Bismuth Chalcogenide Topological Insulators from First Principles: DFT and Beyond

14:40 to 15:20 – Zhong Fang
Topological Insulators and Topological Semimetals

15:20 to 15:50 – Coffee Break

15:50 to 16:30 – Arun Bansil
Electronic Structure and Modeling of Highly Resolved Spectroscopies in Topological Insulators and Other Complex Materials

16:30 to 16:50 – Jürgen Henk
Spin Texture and Magnetism in Pure and Mn-doped Bi_2Te_3

16:50 to 18:00 – Discussion and Poster Highlights

18:00 to 20:00 – Poster Session

Day 2 – January 10, 2012

9:00 to 9:40 – Warren Pickett
Impact of Spin-Orbit Coupling in Transition Metal Pnictides and Oxides

9:40 to 10:20 - Hyoung Joon Choi
Chiral Orbital-Angular-Momentum and Side-Surface Dirac Cone of Topological Insulators

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – Stefan Blügel
Electrically Tunable Quantum Anomalous Hall Effect

11:30 to 12:10 – Joaquin Fernandez-Rossier
Magnetism at the Edges and Surfaces of Topological Insulators

12:10 to 12:30 – Jaroslav Fabian
Spin-Orbit Coupling in Graphene: from Monolayer to Graphite

12:30 to 14:00 – Lunch

14:00 to 14:40 – David Vanderbilt
Orbital Magnetoelectric Coupling and Surface Anomalous Hall Effect

14:40 to 15:20 – Ivo Souza
First-Principles Calculation of the Orbital Magnetoelectric Response

15:20 to 15:50 – Coffee Break

15:50 to 16:30 – Raffaele Resta
A "Topological Marker" in Coordinate Space

16:30 to 16:50 – Pekka Pyykkö
Relativistic Effects in Heavy-Element Chemistry and Physics

16:50 to 17:10 – Hubert Ebert
From Simple Rashba Physics to Topological Insulators: Actual Trends in ARPES

17:10 to 17:30 – Stephan Roche
Exploring Spin-Orbit Coupling Effects in Models of Topological Insulators

19:00 Dinner

Day 3 – January 11, 2012

9:00 to 9:40 – Gustav Bihlmayer
Exploring 2D Topological Insulators under Realistic Conditions by Density Functional Theory

9:40 to 10:20 – Eugene Chulkov
Buried Topological States in a Homological Series of Topological Insulators

10:20 to 10:50 – Coffee Break

10:50 to 11:30 – Stanislav Chadov
Tuning the Topology-Related Properties in Heusler Compounds. First-Principles Study

11:30 to 12:10 – Hai-Jun Zhang
Strongly Interacting Topological Insulators in Actinide Family

12:10 to 12:30 – Binghai Yan
Prediction of Topological Insulators in $TlBiSe_2$ Family of Chalcogenides

12:30 to 14:00 – Lunch

14:00 to 14:20 – George Japaridze
Magnetic Field Induced Quasi Helical Liquid State in a Disordered 1D Electron System with Strong Spin-Orbit Interaction

14:20 to 14:40 – Kyungwha Park
Interface-Induced Magnetism in Topological Insulators Bi_2Te_3 and Bi_2Se_3

14:40 to 15:00 – Closing word

LIST OF PARTICIPANTS

Organizers

Joel Moore (University of California at Berkeley, USA)
David Vanderbilt (Rutgers University, New Brunswick, USA)
Oleg Yazyev (Swiss Federal Institute of Technology Lausanne, Switzerland)

Invited speakers

Arun Bansil (Northeastern University, Boston, USA)
Gustav Bihlmayer (Research Center Julich, Germany)
Stefan Blügel (Research Center Julich, Germany)
Stanislav Chadov (University of Mainz, Germany)
Hyoung Joon Choi (Yonsei University, Seoul, South Korea)
Eugene Chulkov (University of the Basque Country, San Sebastián, Spain)
Andrea Dal Corso (SISSA and CNR-IOM-DEMOCRITOS, Trieste, Italy)
Zhong Fang (Chinese Academy of Sciences, Beijing, China)
Joaquin Fernandez-Rossier (IINL, Braga, Portugal)
Marco Grioni (Swiss Federal Institute of Technology Lausanne, Switzerland)
Zahid Hasan (Princeton University, USA)
Warren Pickett (University of California at Davis, USA)
Raffaele Resta (University of Trieste, Italy)
Ivo Souza (University of the Basque Country, San Sebastin, Spain)
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Contributing participants

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