CECAM Workshop Scientific Report

Workshop: Novel 2D materials: Tuning electronic properties on the atomic scale

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I. Summary

The workshop "Novel 2D materials: Tuning electronic properties on the atomic scale" was held at the University of Bremen, Germany from June 10th to 14th 2013. In total, 76 participants from Belgium, Brazil, Finland, Ireland, Luxemburg, The Netherlands, Portugal, Slovenia, Spain, Sweden, Switzerland, Denmark, France, Germany, UK and US attended the workshop.

The programme consisted of 30 invited lectures, one poster session presenting 37 posters and many events (reception / conference dinner) to allow for informal exchange. The lectures were scheduled to last 40 min, including 5-10 min discussion time. In addition to this extended time for discussion, the chairpersons were instructed to introduce the subject of the session and to actively participate in the discussion. This "Gordon-conference-style" was essential to guarantee a vivid discussion. The organizers ensured that well-established scientists acted as invited speakers and chairpersons.

Concerning the poster session, we accepted only 37 posters to allow for an intense exchange of ideas at each single poster. Here, we encouraged in particular the young scientists to ask questions. The participation of PhD students was supported by partly covering local accommodation costs.

Due to the compact organization and accommodation in one hotel only all participants had to stay together for the whole time of the conference, which additionally enforced the scientific discussion which was mandatory since scientists from various separated fields, i.e. advanced quantum chemistry, many-body perturbation theory, DFT and beyond, scanning probe techniques, optical spectroscopy, ARPES, etc. were attending the meeting to merge ideas and formulate a common goal for future directions and collaborations of theory groups with experimental groups.

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II. Scientific content, main outcome of key presentations, selected discussions

Various sessions have been related to the topics (a) Structure and electronic properties, (b) Novel layered materials, (c) Electrical transport experiments versus theory, (d) Fundamental theory and (e) First-principles calculations, (f) Devices, (g) Electronics contacts, (h) doping. These topics are commonly related to each other. So, extensive attentions and discussions have been stimulated between researchers from different fields.

On the experimental side, progress on several ways to fabricate atomically thin crystals and particularly heterostructures thereof has been reported. Current options include exfoliation, ultrasonication and epitaxial growth. The on-demand production of graphene-hBN heterostructures as well as graphene transition metal dichalcogenide (TMDC) heterostructures by means of exfoliation, subsequent transfer and annealing techniques has been reported by A. Allain (EPF Lausanne) and L. Ponomarenko (U. Manchester). It has been shown by transmission electron microscopy (TEM) that these heterostructure are surprisingly clean: contaminations from the production process are squeezed out of the heterostructures most likely by van-der-Waals interactions. The presentation by U. Kaiser (U. Ulm) further illustrated the potential of TEM for the atomic scale characterization and manipulation of 2d materials. Together with the presentation by A. Krasheninikov (Aalto University) the combination of TEM with first-principles DFT simulations was shown to reveal e.g. atomically precise defect geometries of e.g. single vacancies in graphene as well as their evolution, particularly the clustering of defects, under the electron beam.

Graphene-hBN heterostructures were addressed in several contributions. B. LeRoy (U. Arizona) showed by means of scanning tunneling microscopy the ultimate flatness of graphene-hBN hybrids and demonstrated the formation of moiré structures in this system. These moiré superstructures bring additional length / energy scales to the system by periodic modulations and gapping terms. As shown by L. Ponomarkeno (U. Manchester), these additional length scales have been exploited to realize Hofstaedter's butterfly – an otherwise extremely difficult to observe high magnetic field phenomenon. The issues of secondary Dirac points (M. Mucha-Kruczynski (U. Bath)) and gap opening was addressed by means of tight binding models and first principles theory (P. Kelly (U. Twente) and B. Sachs (U. Hamburg)). It was shown that local sublattice symmetry breaking and average gaps should be distinguished. Depending on the dimensions of the moiré, even local probe experiments will detect average gaps, which can be an order of magnitude smaller than local sublattice symmetry breakings. Scanning tunneling spectroscopy gave an upper limit for average gaps in graphene on h-BN on the order of 1meV. Nevertheless, refined first-principles GW-calculations presented by P. Kelly (U. Twente) showed that many body effects can enhance the tendency for gap opening and lead to local sublattice symmetry breakings on the order of a few 100 meV.

Generally Moiré and many body effects turned out to be one central aspect in many presentations and discussions. At chemically relevant energy scales, moiré structures can control intercalation processes and pattern formation of adsorbates (T. Michely, U. Cologne). Twisted bilayer graphene allows to tune electronic properties in moiré structures down to lowest energies, where additional low energy Dirac fermions can emerge (P. San Jose (U. Madrid)). The topological properties of the quasiparticles, particularly the concept of "valley Chern numbers", were discussed controversially. In any case, it became very clear that moiré effects present a rich toolbox for electronic structure engineering in layered materials.

The long range part of the Coulomb interaction is essentially unscreened in free standing 2d semiconductors and several resulting many body effects were addressed: In transition metal dichalcogenides as well as in hBN many body effects substantially affect quasiparticle energies (particularly energy gaps) due to the long range Coulomb tails as demonstrated by L. Wirtz (U. Luxembourg) and A. Krasheninikov (Aalto University). As for optical excitations, strongly bound excitons can be formed, where binding energies on the order of several 100meV or more nearly compensate GW corrections to quasiparticle energies. Time resolved photoluminescence experiments presented by C. Gadermaier (Jozef Stefan Institute Ljubljana) revealed strongly bound excitons and long lived trions in MoS_2. As pointed out by F. Guinea (ICM Madrid), also low energy charge transport is largely affected by long range Coulomb coupling. In 2d hybrid systems with metallic gates, Coulomb interactions can mediate friction by scattering propagating charge carriers and decrease the conductivity.

Apart from these direct effects, further interactions like electron phonon coupling in 2d materials are highly sensitive to long range Coulomb tails, and require a beyond LDA description, as demonstrated with the issue of Kohn anomalies graphene by L. Wirtz (U. Luxembourg).

The unique possibilities for heavy charge doping of novel 2d materials e.g. by ionic liquid gating (Z. Zhou, U. Detroit) or intercalation (T. Michely, U. Cologne) are highly interesting in the view of many body physics and it remains to be fully explored, how the interplay of Coulomb interactions and doping can be utilized for electronic structure engineering. One impressive example of many body physics at work in 2d materials was demonstration of transient charge density wave melting in TaS2, as observed femtosecond electron diffraction (G. Sciani, U. Hamburg).

On the single particle level, stacking and quantum confinement effects have been proven highly useful for tuning the electronic band gaps in 2d materials, as demonstrated by J. Fernández-Rossier (INL Braga) and A. Kuc (JU Bremen). Clearly the workshop demonstrated that quantum confinement, stacking, Moiré and many body effects combined with doping provide a unique toolbox for engineering electronic properties of 2d materials. Experiment and theory (A. Allain, EPFL, A. Kuc, JU Bremen) agree in recent work that MoS_2, being a 3-atomic layer sandwich, shows similar rippling formation as graphene.

A driving force in the field of 2d materials is clearly the prospects of novel applications including transparent, flexible and printed electronics. While the exploration of the full potential for applications is still at the very beginning, several encouraging examples of novel devices have been presented: A. Allain (EPF Lausanne) showed field effect transistors as well as flash memory devices based on MoS_2 / MoS_2 graphene heterostructres. Prototypal printed electronics (e.g. graphene based sensors) were demonstrated by A. Ferrari (U. Cambridge).

III. Assessment of the results and impact on future direction of the field

The foremost objective of the proposed workshop is to bring together leading and active researchers who work on novel 2-dimensional materials in both experiment and theory and to discuss about possible solutions to improve the quality and tailor the materials based upon computational approaches from physics and chemistry. Aiming for a focused meeting with 70-80 participants we have stimulated exchange, awareness of challenges, approaches and achievements in the respective fields. Moreover, we emphasize to strengthen the links between experimental and computational groups in this fast-developing field and to interconnect current model-type and first-principles descriptions.

The proposed workshop has become a forum to discuss about possible solutions of improving the quality of novel 2D materials and correlating experiment and theory on a highly predictive level. We have been able to achieve the following key objectives:

1) To introduce the fundamentals and application proposals of 2D materials to general audiences. To this goal we have invited renowned scientists to give introductory review talks on the fundamental concepts and progress in this filed. We have attracted more researchers with good knowledge and experience in materials science from the general materials-related community, and could help activate new ideas through knowledge exchange.
2) We have invited active experimental researchers to report their latest progress in novel 2D materials growth/synthesis, characterization and device fabrication. Complementary, computational scientists have introduced newly predicted 2D materials system candidates and described their interesting properties.
3) During the workshop there were many discussions about possible solutions in optimizing the quality and properties of 2D materials and fabricating new devices. We have gathered together researchers from both experiments and computational materials science to better understand current problems in synthesis and application of related 2D systems, determined the priority target of questions to be addressed by state-of-the-art first-principle methods, and discussed possible solutions for magnetic doping and stacking various 2D materials in hetero junctions for construction of novel device functions.
4) The workshop stimulated the interconnection of phenomenological model-type and computational first-principles approaches. Phenomenological theorists and computational materials scientists will foster mutual interactions not only to supply practical parameter inputs for theoretical models, but also to realize interesting proposals using explicit materials.

July 10th 2013

The Organizers