

ISGD-5

5th INTERNATIONAL SYMPOSIUM ON GRAPHENE DEVICES

New Two Dimensional Compounds: Beyond Graphene

In the field of nanosciences, the quest for materials with reduced dimensionality is only at its beginning. While a lot of effort has been put initially on graphene, the focus has been extended in the last past years to functionalized graphene, boron nitride, silicene, and transition metal dichalcogenides in the form of single layers.

Although these two-dimensional compounds offer a larger range of properties than graphene, there is a constant need for new materials presenting equivalent or superior performances to the ones already known.

During this talk, I will present an approach that we have used[1] to discover potential new two-dimensional materials.

This approach corresponds to perform datamining in the Inorganic Crystal Structure Database using simple geometrical criterias, and allowed us to identify nearly 40 new materials that could be exfoliated into two-dimensional sheets. Among this list, we found that Cu₂S could indeed be obtained in the form of quasi-isolated layers[2], with a bandgap of 0.9 eV using the GW approximation.

I will also present some of our recent results[3] concerning the electronic structure of transition metal dichalcogenides bilayers, as well as a recent study[4] of various indium selenides two dimensional compounds.

References:

- [1] S. Lebègue, T. Bjorkman, M. Klintonberg, R. M. Nieminen, and O. Eriksson, Phys. Rev. X. 3, 031002 (2013)
- [2] F. Ben Romdhane, O. Cretu, L. Debbichi, O. Eriksson, S. Lebègue, and F. Banhart, Small 11, 1253 (2015)
- [3] L. Debbichi, O. Eriksson, and S. Lebègue, Phys. Rev. B 89, 205311 (2014)
- [4] L. Debbichi, O. Eriksson, and S. Lebègue, J. Phys. Chem. Letters 6, 3098 (2015)

INVITED SPEAKER:

Dr. S. Lebègue

Equipe Modélisation Quantique, CRM2, Institut Jean Barriol,
CNRS - Université de Lorraine
FRANCE

email: sebastien.lebegue@univ-lorraine.fr