WORKSHOP on the modeling of defects

We are honored to invite you to the following event held under the auspices of the DIM SIRTEQ:

informal mini-workshop about the modeling of point defects,

October 18th 2019, 10h-16h

École Polytechnique, Becquerel amphitheater
https://www.polytechnique.edu/fr/accesetorientation

Contacts: nathalie.vast@polytechnique.edu
jean-francois.roch@ens-cachan.fr

10h00 - Modeling Point Defects for Quantum Information Science

Chris G. Van de Walle

Materials Department, University of California, Santa Barbara, CA 93106-5050, USA
vandewalle@mrl.ucsb.edu

Quantum technologies have recently become a top research priority. Exciting applications are envisioned for computing, communication, and metrology. However, the underlying hardware still requires major development. Point defects in semiconductors and insulators provide a platform that combines the environmental isolation necessary to maintain the coherence of quantum states with the ability to perform electrical and optical manipulation [1]. The nitrogen-vacancy (NV) center in diamond has been widely studied as an individually-addressable quantum system that can be initialized, manipulated, and measured with high fidelity at room temperature. We have performed in-depth first-principles analyses of the NV center in order to elucidate its properties and to predict which centers in other materials might exhibit similarly favorable properties [2,3,4]. I will present an overview of the physics of deep centers, focusing on the characteristics that are key to their performance as "NV-like" centers.

Building on the general methodology for performing point-defect calculations [5], we have developed the capability to predict transition energies and lineshapes associated with the optical transitions that play a central role in the functionality of the defect. Our methodology rigorously addresses the coupling between electrons and phonons during an optical transition, leading to an excellent description of the luminescence band [6,7]. We also model nonradiative transitions [8], which are relevant for the so-called intersystem crossings. These developments enable us to analyze, identify, and predict quantum point defects, as will be illustrated with examples for a number of semiconductors including AlN [4] and BN [9,10].

Work performed in collaboration with A. Alkauskas, D. Awschalom, C. E. Dreyer, L. Gordon, A. Janotti, G. Kresse, J. Lyons, M. Mackoit, J.-X. Shen, M. Turiansky, J. Varley, J. Weber, L. Weston, D. Wickramaratne, and Q. Yan, and supported by DOE and NSF.

Bibliography:

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[8] A. Alkauskas, Q. Yan, and C. G. Van de Walle, Phys. Rev. B **90**, 075202 (2014).

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[10] M. E. Turiansky, A. Alkauskas, L. C. Bassett, and C. G. Van de Walle, Phys. Rev. Lett. **123**, 127401 (2019).

Schedule of the workshop:

Session Theory

10h00 - 10h05: Introduction

10h00 - 10h50: **Chris Van de Walle, University of California, Santa Barbara**
Modeling Point Defects for Quantum Information Science
See abstract above

11h20 -11h40: Vincent Robert, University of Strasbourg
Localized approach to Charge Gap in 1D Hubbard Model

11h55 -12h15: Guido Roma, CEA, Gif-sur-Yvette
Optical Properties of Carbonyl Defects in Polyethylene

Together lunch 12 h 30 - 13h30 at the restaurant of École Polytechnique

Session Experiments

13h30 - 14h00: Jean-François Roch, École Normale Supérieure Paris Saclay
The NV center in diamond as a quantum sensor for high-pressure physics

14h20 - 14h40: Anais Dréau, University of Montpellier
μs-timescale dynamics between NV- and a non-fluorescing state unravelled by time-resolved PL measurements

14h55 - 15h15: Gabriel Hétet, École Normale Supérieure, Paris
Spin-mechanics with particles in Paul traps

15h30 - 16h 00: Final discussions and conclusions