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ETSF Electron-phonon collaboration team workshop

UCLouvain, Louvain-la-Neuve



September 23-25, 2024

COUB16 auditorium
Place Pierre de Coubertin 2,
1348 Louvain-la-Neuve

Organizers

Samuel Poncé
Xavier Gonze
Andrea Marini
Fabio Caruso
Matthieu Verstraete

Program

– Monday –

12:30 - 13:00 Registration & Welcome

13:00 - 13:30 Matthieu Verstraete – *Many body effects in electron phonon coupling: cumulants and anharmonicity*

13:30 - 14:00 Jae-Mo Lihm – *Self-consistent electron-phonon renormalization*

14:00 - 14:30 Yiming Pan – *Real-time simulations of non-thermal lattice dynamics in bulk MoS₂*

14:30 - 15:00 Raveena Gupta – *Exploring electron-phonon interactions in diamond and silicon: insights from spectral analysis*

15:00 - 16:00 Discussion on quasiparticle approximation [X. Gonze]

16:00 - 16:30 Coffee Break

16:30 - 17:00 Francesco Mauri – *Electron-phonon and topology: quantized Born effective charges as probes for the topological phase transition in the Haldane and Kane-Mele models*

17:00 - 17:30 Francesco Macheda – *First principles calculations of dynamical quadrupoles and higher order terms from the density response in large semiconducting and metallic systems*

17:30 - 18:00 Discussion on el-ph in metals [F. Caruso]

– Tuesday –

8:30 - 9:00 Cheol-Hwan Park – *Physical properties of electron relaxons*

9:00 - 9:30 Nakib Protik – *Completing the transport circuit in the interacting electron-phonon system*

9:30 - 10:00 Muralidhar Nalabothula – *Symmetries of excitons: application to exciton-phonon coupling*

10:00 - 10:30 Coffee Break

10:30 - 11:00 Fulvio Paleari – *TBD*

11:00 - 11:30 Silvana Botti – *TBD*

11:30 - 12:30 Discussion on transport and excitons [M. Verstraete]

12:30 - 14:00 Lunch

14:00 - 14:30 Sabyasachi Tiwari – *Quasidegenerate many-body perturbation theory*

14:30 - 15:00 Vasili Vasilchenko – *Recent advances in variational modeling of localized polarons using ABINIT*

15:00 - 15:30 Manuel Engel – *Electron-phonon interactions using the projector-augmented-wave method*

15:30 - 16:00 Coffee Break

16:00 - 16:30 Bartomeu Monserrat – *Efficient Brillouin zone sampling for phonon and electron-phonon calculations*

16:30 - 17:00 Riccardo Reho – *Density functional theory for superconductors: theory and implementation in the SIESTA code*

17:00 - 17:30 Matteo Giantomassi – *GWPT: electron-phonon coupling including many-body effects*

17:30 - 19:00 Discussion on implementation [A. Marini]

19:30 - 22:30 Social Dinner at Brasse-Temps, place des Brabançons 4

– Wednesday –

8:30 - 9:00 Eberhard K. U. Gross – *Non-adiabaticity in electronic and phononic motion: a DFT approach based on the exact factorization*

9:00 - 9:30 Xavier Gonze – *Electron-phonon contribution to the total energy*

9:30 - 10:00 Andrea Marini – *Electron-phonon interaction dynamical screening: insights from exact properties of the three-dimensional homogeneous electron gas*

10:00 - 10:30 Fabio Caruso – *Phonon coherence and decoherence*

10:30 - 11:00 Coffee Break

11:00 - 13:00 Discussion on fundamentals [S. Poncé]

13:00 - 13:15 Final words & Closing