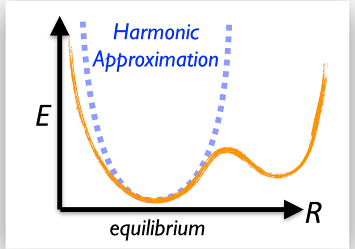
Capturing anharmonic vibrational motion in first-principles simulations



December 6 - December 8, 2021
On-line, hosted by CECAM-HQ

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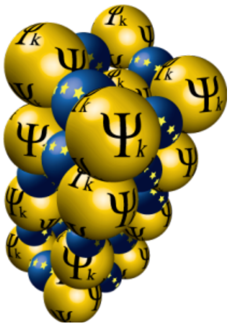

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1. Description

In traditional electronic structure studies, the nuclear motion is typically neglected, albeit having a profound impact on essentially all properties of matter. Even when assuming that the dynamics of electrons and nuclei follows the Born-Oppenheimer approximation, nuclear fluctuations manifest themselves either directly through atomic structural changes in molecules and solids, or indirectly through changes in the electronic structure, due to vibronic coupling. Moreover, the nuclear dynamics defines different response properties of matter, like vibrational excitations, heat transport, diffusion properties, and many more.

Pioneering first-principles studies capturing these effects have relied on the harmonic approximation for the nuclear degrees of freedom or on perturbative expansions thereof, thus accurately capturing *"weak"* anharmonicity at best. These studies were nevertheless successful, being able to shed light on the temperature dependence of electronic band-gaps [1], on intricate vibrational energy reorganization [2], and on the character of vibrational fingerprints of molecules [3]. However, over the last decade, with the increase in accuracy of electronic structure methods and the emergence of materials that combine soft and hard matter, it has become evident that a naïve modeling of the nuclear motion in the harmonic approximation is not sufficiently accurate or even qualitatively incorrect in many cases [4, 5]. This realization has fueled an array of recent methodological developments, ranging from higher-order perturbative methods to novel *ab initio* molecular dynamics approaches – sometimes aided and improved by machine-learning algorithms [6,7]. To cite a few developments where the organizers have been directly involved, one could name novel, fully anharmonic methods for the computational prediction of thermal conductivities [8] and of temperature-dependent electronic properties [9] in solids and the inclusion of quantum anharmonicity in vibrational properties [10,11], both applicable to realistic molecules and solids.

Clearly, the challenges one faces when investigating the vibrational motion vary with the actual material of interest. Within *ab initio* electronic structure simulations, achieving convergence with respect to system size (viz. reciprocal q-points [12]) has been a massive hurdle for inorganic solids, whereas achieving convergence with respect to the configurational entropy of the nuclear degrees of freedom has been equally challenging in organic molecular matter. Ongoing efforts in the scientific community focus on developing more accurate methodologies and on reducing the cost of these simulations. However, the molecular and solid-state communities have few opportunities to meet each other, even if the challenges faced by both when addressing anharmonic nuclear motion are similar. We thus believe it is timely to organize a workshop where expert and prominent code and method developers from these two communities are brought together. We plan a workshop program that will not be aimed at showcasing the participants' achievements, but rather at discussing the nuts and bolts of the methods and implementations – an aspect that often falls short of other presentation formats. Along these lines, we will strongly encourage the participation and involvement of young researchers that are involved in the code development on a day-to-day basis.

Key References

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2. Program

Day 1 - Monday December 6th 2021

- 14:45 to 15:00 - Welcome & Introduction

Novel Methodological Developments 15:00 to 17:30

- 15:00 to 15:30 - Introduction by session leader Feliciano Giustino
- 15:30 to 15:50 - Andrea Marini
  Non-adiabatic classical atomic oscillations within time-dependent density functional perturbation theory
- 15:50 to 16:00 - Discussion
- 16:00 to 16:20 - Federico Grasselli
  The role of invariance principles and topology in the ab initio charge transport of ionic fluids
- 16:20 to 16:30 - Discussion
- 16:30 to 17:30 -**Discussion**: Novel methodological developments *(Chair: Feliciano Giustino)*

Heat Transport 18:00 to 20:30

- 18:00 to 18:30 - Introduction by session leader Christian Carbogno
- 18:30 to 18:50 - Olle Hellman
  Response at finite temperature
- 18:50 to 19:00 - Discussion
- 19:00 to 19:20 - Yi Xia
  Nontrivial role of quartic anharmonicity in lattice heat transfer in binary rocksalt and zincblende compounds
- 19:20 to 19:30 - Discussion
- 19:30 to 20:30 - **Discussion**: Heat transport *(Chair: Christian Carbogno)*

Day 2 - Tuesday December 7th 2021

Electronic Transport and Vibronic Coupling 14:00 to 16:30

- 14:00 to 14:30 - Introduction by session leader Ivana Savic
- 14:30 to 14:50 - Ion Errea
  Quantum anharmonic effects on the superconducting properties of high-Tc hydrides
- 14:50 to 15:00 - Discussion
- 15:00 to 15:20 - Samuel Poncé
  Ab initio calculation of carrier mobility in bulk and low-dimensional materials
- 15:20 to 15:30 - Discussion
- 15:30 to 16:30 - **Discussion**: Electronic transport and vibronic coupling *(Chair: Ivana Savic)*

Thermodynamics and Free Energies 17:00 to 19:30

- 17:00 to 17:30 - Introduction by session leader Graeme Day
- 17:30 to 17:50 - Tilmann Hickel
- 17:50 to 18:00 - Discussion
- 18:00 to 18:20 - Johannes Hoja

Anharmonic vibrations for molecular crystals via dimer embedding and vibrational perturbation theory
- 18:20 to 18:30 - Discussion
- 18:30 to 19:30 - **Discussion**: Thermodynamics and free energies *(Chair: Graeme Day*)

Poster Session @ Gather.town

- 20:00 to 21:00 - Poster session

Day 3 - Wednesday December 8th 2021

Anharmonic Effects in Vibrational Spectroscopy 15:00 to 17:30

- 15:00 to 15:30 - Introduction by session leader Mariana Rossi
- 15:30 to 15:50 - Luber Sandra
  Going beyond the harmonic approximation using density functional theory-based molecular dynamics
- 15:50 to 16:00 - Discussion
- 16:00 to 16:20 - Carolin König
  Embedded vibrations for tailored anharmonic spectra of complex systems
- 16:20 to 16:30 - Discussion
- 16:30 to 17:30 - **Discussion**: Anharmonic effects in vibrational spectroscopy *(Chair: Mariana Rossi)*

Machine-Learning Aided Approaches 18:00 to 20:30

- 18:00 to 18:30 - Introduction by session leader Tom Purcell
- 18:30 to 18:50 - Fredrik Eriksson
  Regularized regression extraction and application of higher order force constants.
- 18:50 to 19:00 - Discussion
- 19:00 to 19:20 - Venkat Kapil
  The first-principles phase diagram of monolayer nanoconfined water
- 19:20 to 19:30 - Discussion
- 19:30 to 20:30 - **Discussion**: Machine-learning aided approaches *(Chair: Tom Purcell)*
- 20:30 to 20:40 - Closing word

3. Abstracts

Ab initio calculation of carrier mobility in bulk and low-dimensional materials

Samuel Poncé[1], Francesco Macheda[2], Nicola Bonini[2], Elena Roxana Margine[3], Miquel Royo[4], Massimiliano Stengel[4], Marco Gibertini[5], Nicola Marzari[6], Feliciano Giustino[7]
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In this talk, I will present recent advances in the field of ab initio calculations of drift and Hall carrier mobilities in bulk materials and 2D materials, relying on exact electrostatic.

In particular, I will present results for the transport properties of 10 simple bulk semiconductors and MoS_2 monolayers within the framework of the Boltzmann transport equation.

These calculations require extremely fine sampling of the Brillouin Zone which is made possible at an affordable computational cost through the use of efficient Fourier-Wannier interpolation of the electron-phonon matrix elements as implemented in the EPW code which also includes the exact treatment of long-range 2D and 3D dipole and quadrupole contributions.

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Anharmonic vibrations for molecular crystals via dimer embedding and vibrational perturbation theory

Johannes Hoja, A. Daniel Boese
University of Graz, Austria

Accurate vibrational properties are crucial for the modeling of molecular crystals, especially for crystal structure predictions, where numerous energetically similar polymorphs have to be ranked according to their Gibbs free energy [1]. However, routine calculations of many practically relevant molecular crystals are essentially limited to density functional theory (DFT) calculations employing mainly the harmonic approximation. A first step towards anharmonic effects for molecular crystals is the quasi-harmonic approximation, which allows the description of thermal expansion of the unit cell, while the phonons at a particular volume are still described in a harmonic fashion [2, 3].

Herein, we present a methodology for anharmonic vibrational properties, which is based on a subtractive embedding scheme developed for improving electronic energies and geometries [4]. In this approach, the full periodic system is calculated within the harmonic approximation, and contributions of monomers and dimers within a certain cutoff distance are obtained via second-order vibrational perturbation theory (VPT2) [5]. First, we benchmark the accuracy of VPT2 frequencies calculated with CCSD(T) based on a diverse set of small molecular dimers with representative intermolecular interactions. Next, we discuss simple approaches for dealing with problematic large-amplitude motions. Finally, we compare the CCSD(T) results with DFT calculations and utilize the above-mentioned embedding approach for small molecular crystals.

[1] J. Hoja, H. Ko, M. Neumann, R. Car, R. DiStasio, A. Tkatchenko, Sci. Adv., ***5****, (2019)*
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Embedded vibrations for tailored anharmonic spectra of complex systems

Carolin König

Leibniz University Hannover, Germany

Many vibrations in biomolecular systems are known to be anharmonic. This holds for example for vibrations affected by hydrogen bonds. Furthermore, quantum effects can be important for the required accuracy. A full anharmonic quantum-mechanical treatment is, however, computationally clearly out of reach. Fortunately, we are hardly interested in the full spectrum, but rather in certain spectral signatures. This means that tailored methods that focus the computational effort on the features of interest are highly desired [1].

In this contribution, I will discuss possible ways tailor anharmonic vibrational wave function calculations for vibrational spectra calculation. This includes the choice of vibrational coordinates as well as vibrational embedding methods. I will show that vibrational self-consistent field (VSCF) and certain parameterizations of vibrational coupled cluster (VCC) are very well suited for subset approaches and how subset approaches can be applied within vibrational response calculations to tailor computations to particular spectroscopic features of interest.

*[1] C. König, Int. J. Quantum. Chem., **121**, (2020)*

Going beyond the harmonic approximation using density functional theory-based molecular dynamics

Luber Sandra

University of Zurich, Switzerland

In this talk, I will give an overview about our work on dynamic methods for spectroscopy [1]. I will describe our approaches for efficient calculation of Infrared spectra for periodic systems [2] using subsystem density functional theory (DFT) as well as Raman [3] and sum frequency generation [4] spectra using density functional perturbation theory. Moreover, pioneering Raman optical activity spectra for the investigation of chiral compounds using DFT-based molecular dynamics have been presented [5]. In addition, I will give an overview about our developments using real time time-dependent density functional theory for the study of absorption and vibrational spectra for (chiral) compounds in the gas and condensed phase [6- 10].

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Non-adiabatic classical atomic oscillations within time-dependent density functional perturbation theory

Andrea Marini, Fulvio Paleari

CNR, Italy

Static Density Functional Perturbation Theory is widely used to calculate phonon frequencies from first principles. In this approach the response of the electrons to the atomic displacements are treated adiabatically and no retardation is included.

In this talk I will propose an extension of Static Density Functional Perturbation Theory which takes into account retardation effects in the electronic response. I will I discuss the case where at a given reference time t_0 the atoms are taken away of their equilibrium positions and leave oscillating starting from an initial position and speed.

I will demonstrate how the retarded oscillation of the electrons dress the phonon energies keeping them real. I will exactly demonstrate that, based on this theory, classical atomic oscillations never decay.
The present results question the common belief that a dynamical extension of Density Functional Perturbation Theory can describe phonon widths representing a valid alternative to the expensive Many-Body Perturbation Theory calculations.
I will also discuss the connection between the non-adiabatic Density Functional Perturbation Theory and the diagrammatic Many-Body perturbation theory.

Nontrivial role of quartic anharmonicity in lattice heat transfer in binary rocksalt and zincblende compounds

Yi Xia, Vinay Hegde, Koushik Pal, Xia Hua, Dale Gaines, Shane Patel, Jiangang He, Muratahan Aykol, Chris Wolverton
Northwestern University, United States

Heat conduction plays a critical role in the performance of microelectronic and energy-conversion devices. To meet the cooling demands of microprocessors and the efficiency of energy converters, researchers are particularly interested in identifying semiconducting materials with extreme thermal conductivities. Surprisingly, these have been discovered in binary cubic compounds. Therefore, a comprehensive understanding of their underlying heat transfer mechanism is of fundamental importance, yet it remains elusive because of the challenges arising from explicitly treating higher-order anharmonicity. Using compressive sensing lattice dynamics, we investigate the lattice heat transfer in a comprehensive set of binary rock salt and zincblende compounds, with a particular focus on unraveling the impacts of quartic anharmonicity. We find that including quartic anharmonicity always decreases the lattice thermal conductivity in zincblendes but can increase or decrease the conductivity in rock salts, owing to the countervailing effects on finite-temperature-induced shifts in phonon frequencies and scattering rates. Among notable examples, we show that four-phonon scattering is unprecedentedly strong in the zincblende mercury telluride, and strong phonon scattering leads to a possible breakdown of the phonon gas model in the rock salt silver chloride. Our results pave the way for an in-depth understanding of heat transfer in a broad class of technologically important compounds, which may guide future engineering.

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Quantum anharmonic effects on the superconducting properties of high-Tc hydrides

Ion Errea
University of the Basque Country, Spain

In the last six years superconducting temperatures above 200K have been measured in several hydrogen-based compounds at megabar pressures, breaking the Tc records set by the cuprates. Despite it is clear now that hydrogen-based compounds can be high-Tc superconductors, the challenge now is to understood if this type of compounds can keep their outstanding superconducting properties at low, even ambient, pressures.
In this talk, I will show that this type of superconductors is subject to huge lattice quantum effects and, consequently, anharmonicity. Their superconducting properties cannot be understood from first-principles unless quantum anharmonic effects are considered in the calculations. Moreover, it seems that quantum anharmonic effects can make stable high-Tc compounds at much higher pressures than expected in the standard classical harmonic approximation, bringing hopes for the discovery of new compounds at low pressures.
I will review how we perform calculations of the vibrational spectra and the electron-phonon coupling in this strongly anharmonic limit within the stochastic self-consistent harmonic approximation (sscha.eu) method.

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Regularized regression extraction and application of higher order force constants.

Fredrik Eriksson, Erik Fransson, Paul Erhart
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Higher order force constants (FCs) play a key role in lattice dynamics when studying e.g. conductivity and stabilization. Typically, FCs have been extracted using the finite displacement method which however suffers from poor scaling properties. Fortunately, during the last decade regression-based approaches have gained traction. This means that force constants can be parametrized like an empirical potential via regularized regression and feature selection. However, the convergence behavior of these techniques, in particular with respect to thermodynamic properties is not well understood.

Thus, we'll present some analysis of the efficacy and efficiency of several state-of-the-art regression and feature selection methods in the context of FC extraction and the prediction of different thermodynamic properties. Generic feature selection algorithms such as recursive feature elimination with ordinary least-squares (OLS), automatic relevance determination regression, and the adaptive least absolute shrinkage and selection operator can yield physically sound models for systems with a modest number of degrees of freedom. For large unit cells with low symmetry and/or high-order expansions they come, however, with a non-negligible computational cost that can be more than two orders of magnitude higher than that of OLS. In such cases, OLS with cutoff selection provides a viable route for both second-order FCs in large low-symmetry unit cells and high-order FCs in low-symmetry systems. While regression techniques are thus very powerful, they require well-tuned protocols. We hope to provide some guidelines for the design of protocols that are readily usable, e.g., in high-throughput and materials discovery schemes. Furthermore, efficient regression allows for construction of interatomic potentials based on higher order force constants. This functional form can sometimes be more advantageous compared to generic ML potentials and opens up for interesting comparisons between BTE and GK.

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Response at finite temperature

Ole Hellman
Visitor in Applied Physics and Materials Science at the California Institute of Technology (Caltech), United States

We present recent developments using the temperature dependent effective potential technique (TDEP) to model vibrational properties of materials. The technique relies on explicitly temperature-dependent model Hamiltonians to capture all orders of non-harmonic effects. Recent developments include determination of high order Raman spectra and thermal transport based on Green-Kubo formalism in contrast with the more established Boltzmann transport. In addition, we will present a generalization of the TDEP technique to magnetic systems.

The first-principles phase diagram of monolayer nanoconfined water

Venkat Kapil[1], Christoph Schran[1], Andrea Zen[2], Ji Chen[3], Chris J. Pickard[1], Angelos Michaelides[1]
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Water in nanoscale cavities is ubiquitous and of central importance to everyday phenomena in geology and biology, and at the heart of current and future technologies in nano-science. A molecular-level picture of the structure and dynamics of nano-confined water is a prerequisite to understanding and controlling the behavior of water under confinement. Here we explore a monolayer of water confined within a graphene-like channel [1] using a framework that combines developments in high-level electronic structure theory [2], machine learning [3], and statistical sampling [4]. This approach enables a treatment of nano-confined water at unprecedented accuracy. We find that monolayer water exhibits surprisingly rich and diverse phase behavior that is highly sensitive to temperature and the van der Waals pressure acting within the nano-channel. Monolayer water exhibits numerous molecular ice phases with melting temperatures that vary by over 400 degrees in a non-monotonic manner with pressure. In addition, we predict two unexpected phases: a ”hexatic-like” phase, which is an intermediate between a solid and a liquid, and a superionic phase with a high electrical conductivity exceeding that of battery materials. Our work suggests that nano-confinement could be a promising route towards superionic behavior at easily accessible conditions.

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The role of invariance principles and topology in the ab initio charge transport of ionic fluids

Federico Grasselli[1], Stefano Baroni[2], Paolo Pegolo[3]
[1]EPFL, Switzerland
[2]SISSA and CNR-IOM, Italy
[3]SISSA, Italy

In my talk, I will show how to combine a recently-formulated gauge-invariance principle of transport coefficients [1,2] with arguments from charge-transport quantization [3] to tackle the problem of ab initio charge transport in materials displaying an electronic band gap, like ionic fluids. By leveraging the Green Kubo theory of linear response, I will prove that the same static electrical conductivity is obtained if the time-dependent Born charge tensors, entering the definition of the ab initio charge flux according to the modern theory of polarization (MTP), are replaced by the time-independent integer oxidation numbers of the atoms [4,5]. Besides providing an alternative method to compute the ab initio electrical conductivity with no need for MTP calculations, this result offers a topology-based definition of oxidation numbers in disordered materials, as I show through numerical experiments on molten potassium chloride. I finally discuss non-stoichiometric systems, where quantized charge transport may occur without a net ionic displacement [6].

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4. Participant list

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