Author's bibliography of Luigi Cigarini

Total number of citations: 26 (Web of Science)

h-index: 4 (Web of Science)

Total number of citations excluding self-citations: 17 (Web of Science)

1. **-,-,-,-,-. "Giant Linear and Nonlinear Excitonic Responses in an Atomically Thin Indirect Semiconductor Nitrogen Phosphide". *The Journal of Physical Chemistry C*, 125(23), 12738–12757 (2021). Corrected in DOI: 10.6084/m9.figshare.19617699 and in www.luigicigarini.net/Corr_JPCC_Supp_Logical.pdf.**

   IF at time of publication: 4.188 (Scopus 4-Year Impact Factor)

   Total number of citations: 7 (Web of Science)
   Total number of citations excluding self-citations: 4 (Web of Science)

   In this work exceptionally large exciton-driven responses of the examined system are demonstrated. The influence of lattice vibrations on the absorption spectra unfolds strong electronic couplings to both LA and ZO-TO phonon modes. All the linear process analyses were computed using a fully *ab initio*-based G_0W_0 + Bethe–Salpeter equation approach that also includes the electron–phonon self-energies. The nonlinear processes were instead obtained using a real-time *ab initio* process flow after creating a coupling between the time-dependent external electric field and the correlated electrons within the modern theory of polarization and the same electron–hole interaction level.

   The contribution is outlined in:
   https://www.luigicigarini.net/Corr_JPCC_Supp_Logical.pdf.
   Luigi Cigarini performed part of the computational simulations relevant to stability and vibrational structure, fully analyzed the results relevant to stability and vibrational structure, fully wrote the sentences of the text relevant to stability and vibrational structure, participated in revision of the text.

2. **Luigi Cigarini, Michal Novotný and František Karlický. "Lattice dynamics in the conformational environment of multilayered hexagonal boron nitride (h-BN) results in peculiar infrared optical responses". *Physical Chemistry Chemical Physics*, 23(12), 7247-7260 (2021). Corrected in DOI: 10.6084/m9.figshare.19619889 and in DOI: 10.6084/m9.figshare.21941294.**

   IF at time of publication: 3.644 (Scopus 4-Year Impact Factor)

   Total number of citations: 1 (Web of Science)
   Total number of citations excluding self-citations: 1 (Web of Science)

By taking advantage of the geometrical and chemical nature of h-BN, we show how simple structural models, based on shortened interplanar distances, can produce effective charge densities. Accounting these in the non-analytical part of the lattice dynamical description makes it possible to access information about the composition of differently stacked variants in experimental samples characterized by infrared spectroscopy. The results are obtained by density functional theory and confirmed by various functionals and pseudopotential approximations. Even though the method is shown using h-BN, the conclusions are more general and show how effective dielectric models can be considered as valuable theoretical pathways for the vibrational structure of any layered material.

Contribution: Luigi Cigarini participated in conceived the initial idea, performed most of the computational simulations, fully analyzed the results, fully conceived the interpretative model, wrote the first version of the text, fully created all the visual graphics of the main paper and most of the supportive ones and participated in the final revision of the text.

3. **Luigi Cigarini, Alice Ruini, Alessandra Catellani and Arrigo Calzolari. "Conflicting effect of chemical doping on the thermoelectric response of ordered PEDOT aggregates". *Physical Chemistry Chemical Physics*, 20(7), 5021-5027 (2018).**

   IF at time of publication: 3.942 (Scopus 4-Year Impact Factor)

   Total number of citations: 4 (Web of Science)
   Total number of citations excluding self-citations: 4 (Web of Science)

   Poly(3,4-ethylenedioxythiophene) (PEDOT) semiconductor plays a relevant role in the development of organic thermoelectric (TE) devices for low-power generation. While dopant counterions are usually needed to provide electrical conductivity, their overall effects on the thermoelectric response of the systems are unknown and uncontrolled. Here, we present a first principles study of the electronic and thermal transport of PEDOT crystalline assemblies, specifically analyzing the role played by tosylate dopants on the thermoelectric figure of merit of the doped system. Our results demonstrate that, beside the desired charging effect, the presence of dopants impacts the bulk configuration by inflating the packing structure and worsening the intrinsic transport properties of the PEDOT host. This provides a rationale for the necessity of controlling the optimal amount and the structural incorporation of dopant in order to maximize the thermoelectric response of organic materials.

   Contribution: Luigi Cigarini conceived the initial idea, performed all the computational simulations, fully performed guided analysis of the results, participated in conceiving the interpretative model, wrote the first version of the paper.

4. **Luigi Cigarini, Alice Ruini, Alessandra Catellani and Arrigo Calzolari. "Thermoelectric figure of merit of polymeric systems for low-power generators". *Journal of Physics D: Applied Physics*, 50(39), 395502-395509 (2017).**

   IF at time of publication: 2.857 (Scopus 4-Year Impact Factor)

Total number of citations: 3 (Web of Science)
Total number of citations excluding self-citations: 2 (Web of Science)

Using calculations from first principles and the Landauer approach for both electron and phonon carriers, we study the thermoelectric figure of merit *zT* of three representative and largely used polymer chains, namely poly(3,4-ethylenedioxythiophene), polyaniline and polyfluorene. Our results provide an upper-limit estimate of *zT*, due to the intrinsic electronic and vibrational properties of the selected compounds, and pave the way to a microscopic understanding of the mechanisms that affect their electronic and transport characteristics in terms of structural distortions and chemical doping.

Contribution: Luigi Cigarini participated in conceiving the initial idea, performed all the computational simulations, participated in the analysis of the results, fully created all the visual graphics, wrote the first version of the paper and participated in revision of the text.

5. **Mauro Sassi, Matteo M. Salamone, Luca Beverina, Gianluca Longoni, Claudio Fontanesi, Davide Vanossi, Luigi Cigarini and Riccardo Ruffo. "An Integrated Theoretical/Experimental Study of Quinolinic–Isoquinolinic Derivatives Acting as Reversible Electrochromes". *Materials*, 10(7), 802-815 (2017).**

IF at time of publication: 2.467 (Clarivate Analytics)

Total number of citations: 0 (Web of Science)
Total number of citations excluding self-citations: 0 (Web of Science)

Density functional theory (DFT) calculations are exploited in order to rationalize the correlation between the molecular structure, the functional groups' electronic properties, and the electrochemical behavior of a series of compounds, featuring an ethenylic bridge and quinoline and isoquinoline end capping units, possessing systematically varied substitution patterns. It is shown that the molecular planarity (i.e. ring/ring π conjugation) plays a major role in defining the mechanism of the electrochemical charge transfer reaction, while the substituent's nature has an influence on the LUMO energy.

Contribution: Luigi Cigarini performed all the computational simulations and participated in the analysis of the results of the theoretical part of the work.

6. **Davide Vanossi, Luigi Cigarini, Andrea Giaccherini, Enrico Da Como and Claudio Fontanesi. "An integrated experimental/theoretical study of structurally related poly-thiophenes used in photovoltaic systems". *Molecules*, 21(1), 110-119 (2016).**

IF at time of publication: 2.861 (Clarivate Analytics)

Total number of citations: 7 (Web of Science)
Total number of citations excluding self-citations: 4 (Web of Science)

In this work, a series of eight thiophene-based polymers (exploited as "donors" in bulk heterojunction photovoltaics cells), whose structures were designed to be suitably tuned with the electronic characteristics of the [6,6]-Phenyl C61 butyric acid methyl ester (PCBM), is considered,. The electronic properties of the mono-, di-, trimeric oligomers are reckoned (at the Hartree-Fock and DFT level of the theory) and compared to experimental spectroscopic and electrochemical results. Indeed, electrochemical and spectroscopic results show a systematic difference whose physical nature is assessed and related to the exciton (electron-hole) binding energy (J e , h). The critical comparison of the experimental and theoretical band gaps, i.e., the HOMO-LUMO energy difference, suggests that electrochemical and DFT values are the most suited to being used in the design of a polythiophene-based p-n junction for photovoltaics.

Contribution: Luigi Cigarini performed most of the computational simulations, participated in the analysis of the results and in the graphical visualizations.

7. **Luigi Cigarini, Davide Vanossi, Federica Bondioli and Claudio Fontanesi. "A novel synthetic strategy for magnetite-type compounds. A combined experimental and DFT-computational study". *Physical Chemistry Chemical Physics*, 17(32), 20522-20529 (2015).**

   IF at time of publication: 4.639 (Scopus 4-Year Impact Factor)

   Total number of citations: 4 (Web of Science)
   Total number of citations excluding self-citations: 2 (Web of Science)

   The dynamics of the early stage reaction between benzyl alcohol and Fe(acetylacetonate)$_3$ is studied by exploiting the Dynamic Reaction Coordinate (DRC) approach, at the PBE0/6-31G* level of theory. Analysis of the DRC trajectory provides a detailed molecular insight into the catalytic effect observed in the acidic reaction environment, compared to the neutral one. The presence of an additional proton in the reaction system, meant to simulate an acidic reaction environment, dramatically affects the reaction path: both by decreasing the activation energy of the complex dissociation and leading to the formation of acetone.

   Contribution: Luigi Cigarini performed part of the computational simulations, participated in the analysis of the results, fully created all the visual graphics, and participated in writing the first version of the text.

Conference contributions

Posters (The name of the author who presented the poster is underlined)

- Miroslav Kolos, Luigi Cigarini, Rekha Verma, František Karlický, Sitangshu Bhattacharya, “Electron-phonon coupling effects and temperature dependence of the excitonic response in a single layer hexagonal nitrogen phospide NP”, 14-18 June 2021, 2021 Virtual School on

Electron-Phonon Physics and the EPW code.

- Luigi Cigarini, Michal Novotný, František Karlický, “Understanding the lattice dynamics of multilayered h-BN: peculiar infrared optical responses”. 4th Users' Conference of IT4Innovations, 5 November 2020, Virtual conference.

- Luigi Cigarini, Michal Novotný, František Karlický, “Understanding the lattice dynamics of multilayered h-BN: peculiar infrared optical responses”. Graphene 2020, 19-23 October 2020, Virtual conference.

- Luigi Cigarini, Michal Novotný, František Karlický, “Understanding the stacking interaction and conformational environment of 3D h-BN: beyond the LDA approach”. Computational School on Electronic Excitations in Novel Materials Using the Yambo Code, 27-31 January 2020, Trieste, Italy.

- Michal Novotný, Luigi Cigarini, František Karlický, “Structural and vibrational properties of boron nitride”. ICAMM Rennes 2019 - International Conference on Advanced Materials Modelling, 1-3 July 2019, Rennes, France.

- Luigi Cigarini, Alice Ruini, Alessandra Catellani, Arrigo Calzolari, “First-principles calculation of the thermoelectric figure of merit of polymeric systems”. ECT 2016 - 14th European Conference on Thermoelectrics, 20-23 September 2016, Lisbon, Portugal.

- Luigi Cigarini, Alice Ruini, Alessandra Catellani, Arrigo Calzolari, “First-principles calculation of the thermoelectric figure of merit of polymeric systems”. SINFO III 2016 - Surfaces, Interfaces and Functionalization Processes in Organic Compounds and Applications, 27-29 June 2016, Naples, Italy.

- Davide Vanossi, Luigi Cigarini, Andrea Giaccherini, Massimo Innocenti, Claudio Fontanesi, “Band gap revised: A computational study of structurally related poly-thiophenes for photovoltaics”. ENERCHEM 2016 - Congress of the Interdivisional Group of the Italian Chemical Society on Chemistry of Renewable Energies, 18-20/02/2016, Florence, Italy.

- Claudio Fontanesi, Davide Vanossi, Luigi Cigarini, Eleonora Ussano, Giovanni Valenti, Matteo Iurlo, Francesco Paolucci, Massimo Marcaccio, “A Theoretical Study on the Electrochemical Synthesis of Seizable PAH Nanostructures for ECL”. ECL 2014 - International meeting on Electrogenerated Chemiluminescence, 07-10 September 2014, Bertinoro, Italy.

- Claudio Fontanesi, Davide Vanossi, Luigi Cigarini, Adele Mucci, Enrico Da Como, “A DFT Computational Study of Structurally Related Poly-Thiophenes Used in Photovoltaic Systems”. WINTER MODELING 2014, 13-14 March 2014, Modena, Italy.