## Rozzi Ca

## List of Publications by Year in descending order

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octopus: a tool for the application of time-dependent density functional theory. Physica Status Solidi
(B): Basic Research, 2006, 243, 2465-2488. (B): Basic Research, 2006, 243, 2465-2488.

2 Coherent ultrafast charge transfer in an organic photovoltaic blend. Science, 2014, 344, 1001-1005.
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3 Exact Coulomb cutoff technique for supercell calculations. Physical Review B, 2006, 73, .
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Quantum coherence controls the charge separat
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Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in
extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.
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Tracking the coherent generation of polaron pairs in conjugated polymers. Nature Communications,
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Photoexcitation of a Light-Harvesting Supramolecular Triad: A Time-Dependent DFT Study. Journal of
$7 \quad$ Physical Chemistry B, 2009, 113, 5345-5349.

Quenching of Majority-Channel Quasiparticle Excitations in Cobalt. Physical Review Letters, 2002, 88,
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9 Electron-Electron Interactions in Artificial Graphene. Physical Review Letters, 2012, 108, 246803.
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10 <i>Ab Initio</i>Simulation of Optical Limiting: The Case of Metal-Free Phthalocyanine. Physical Review
Letters, 2014, 112, 198303.

> Quantum modeling of ultrafast photoinduced charge separation. Journal of Physics Condensed
> Matter, 2018, 30, 013002.

Ab initioFermi surface and conduction-band calculations in oxygen-reducedMoO3. Physical Review B, 2003, 68, .

Understanding real-time time-dependent density-functional theory simulations of ultrafast
laser-induced dynamics in organic molecules. Journal of Chemical Physics, 2020, 153, 054106.

14 Intermolecular conical intersections in molecular aggregates. Nature Nanotechnology, 2021, 16, 63-68.
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15 Charge Separation Dynamics and Optoâ€Electronic Properties of a Diaminoterephthalateâ€C<sub>60</sub>
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A Diaminoterephthalateâ€"C60 Dyad: A New Material for Optoelectronic Applications. Synthesis, 2015, 47,
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Exact Coulomb cutoff technique for supercell calculations in two dimensions. Physical Review B,
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Modeling solvation effects in real-space and real-time within density functional approaches. Journa
of Chemical Physics, 2015, 143, 144111.

Nonequilibrium Solvent Polarization Effects in Real-Time Electronic Dynamics of Solute Molecules
20 Subject to Time-Dependent Electric Fields: A New Feature of the Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2019, 15, 2306-2319.
Band-structure effects in the core-level photoemission spectra of NiO. Physical Review B, 2000, 62,

R4774-R4777. $\quad$| 3.2 |
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A listening experiment comparing the timbre of two Stradivari with other violins. Journal of the Acoustical Society of America, 2022, 151, 443-450.

27 Light tuning of the image potential state electron-electron interactions. Surface Science, 2008, 602,
2983-2988.

28 Roadmap on bio-nano-photonics. Journal of Optics (United Kingdom), 2021, 23, 073001.
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Theoretical simulation of core-level photoemission in transition-metal oxides. Physical Review B,
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Correlation effects on the electronic properties of Bi 2 Sr 2 CaCu 2 O . Journal of Physics and Chemistry
30 of Solids, 2006, 67, 286-288.
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Density functional approach to the band gaps of finite and periodic two-dimensional systems. Physical
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Indoor noise level measurements and subjective comfort: Feasibility of smartphone-based participatory experiments. PLoS ONE, 2022, 17, e0262835.
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Quantum coherence controls the charge separation in a prototypical artificial light harvesting
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Spin dependent many-body effects in the photoemission of Co. Journal of Electron Spectroscopy and

38 Prototyping Ultrafast Charge Separation by Means of Time-Dependent Density Functional Methods. , 2018, , 1-19.

Quantum coherence controls the charge separation in a prototypical artificial light harvesting system. , 2012, , .

