

Nektarios N. Lathiotakis

Senior researcher

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EDUCATION

- PhD in Physics, Physics Department, University of Crete (1997)
- Masters in Condensed Matter Physics, Physics Dept., University of Crete (1993)
- Diploma in Physics, Physics Department, University of Crete (1990)

RESEARCH AND TEACHING APPOINTMENTS

2013- : Senior Researcher (B), TCPI/NHRF

Nov 2014-Nov 2015 : Visiting Researcher, Max Planck Institut für Mikrostrukturphysik, Halle, Germany (on sabbatical)

2007-2012: Associate Researcher (C), TCPI/NHRF

2001-2007: Postdoctoral Researcher, Fachbereich Physik, Freie Universität, Berlin, Germany

2000-2001: Postdoctoral Researcher, Institut für Theoretische Physik, Universität Würzburg, Germany

1997-2000: Postdoctoral Researcher, H. H. Wills Physics Lab., Univ. of Bristol, U.K.

MAIN RESEARCH INTERESTS

- Theoretical Materials Science, Electronic Structure
- Density Functional Theory, Density Matrix Functional Theory
- DFT for Superconductors
- Structural, Mechanical, Electronic and magnetic properties of finite and periodic systems
- Time Dependent - DFT, optical spectrum of molecular systems
- Structural, elastic and electronic properties of 2D materials

HONORS – AWARDS - FUNDING

- Cost Action MP1306 (EUSpec): "Modern Tools for Spectroscopy on Advanced Materials", Member of the Management Committee (2015-2018).
- Enabling Excellence, European Training Network (ETN): "Graphene-based nanomaterials for touchscreen technologies", Member of NHRF team (2015-2019).
- GSRT-Kripis: "Novel Multifunctional Nanostructured Materials and Devices", POLYNANO – 447963, Coordinator of the theory research subproject (2012-2015).
- Thales, GRAPHENECOMP, member of the research team, 1-2-2012/31-8-2015
- Deutsche Forschungsgemeinschaft, SPP-1145 (2003-2005) and (2005-2007)
- TMR-Network, Post-doctoral Fellow (1997-2000) and (2000-2003)
- IESL-FORTH Postgraduate Fellowship (1991-1996), Greek State Post-graduate fellowship (EMY) (1991-1996)

PUBLICATIONS - PRESENTATIONS

- 58 articles in refereed journals, 3 articles in conference proceedings, 1355 citations, h-index: 22 (Feb 2017); ResearcherID: [C-5647-2008](#)
- 54 presentations, 42 talks, 23 invited talks (Feb 2017).

SELECTED RECENT PUBLICATIONS

1. "Electron transfer through organic molecular wires: A theoretical study", N. N. Lathiotakis, G. Theodorakopoulos, I. D. Petsalakis, [Chem. Phys. Lett. 667, 45 \(2017\)](#).
2. "Conditions for Describing Triplet States in Reduced Density Matrix Functional Theory", I. Theophilou, N. N. Lathiotakis, N. Helbig, [J. Chem. Theory Comput. 12, 2668 \(2016\)](#).
3. "Tailoring the spacer type and length in push-pull chromophores. Insights from a systematic theoretical study", [Chem. Phys. Lett. 653, 178 \(2016\)](#).
4. "Graphene allotropes under extreme uniaxial strain: an ab initio theoretical study", Z. G. Fthenakis, N. N. Lathiotakis, [Phys. Chem. Chem. Phys. 17, 16418 \(2015\)](#).
5. "Spectrum for Nonmagnetic Mott Insulators from Power Functional within Reduced Density Matrix Functional Theory", Y. Shinohara, S. Sharma, S. Shallcross, N. N. Lathiotakis, E. K. U. Gross, [J. Chem. Theory Comput. 11, 4895 \(2015\)](#).
6. "Doping induced metal-insulator phase transition in NiO - a reduced density matrix functional theory perspective", Y. Shinohara, S. Sharma, J. K. Dewhurst, S. Shallcross, N. N. Lathiotakis, E. K. U. Gross, [New J. Phys. 17, 093038 \(2015\)](#).
7. "Generalized Pauli constraints in reduced density matrix functional theory", I. Theophilou, N. N. Lathiotakis, M.A.L. Marques, N. Helbig, [J. Chem. Phys. 142, 154108 \(2015\)](#).
8. "Quasi-particle energy spectra in local reduced density matrix functional theory", N. N. Lathiotakis, N. Helbig, A. Rubio, N. I. Gidopoulos, [J. Chem. Phys. 141, 164120 \(2014\)](#).

9. "Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations", N. N. Lathiotakis, N. Helbig, A. Rubio, N. I. Gidopoulos, [Phys. Rev. A 90, 032511 \(2014\)](#).
10. "In-plane force fields and elastic properties of graphene", G. Kalosakas, N. N. Lathiotakis, C. Galiotis, K. Papagelis, [J. Appl. Phys. 113, 134307 \(2013\)](#).
11. "Constraining density functional approximations to yield self-interaction free potentials", N. I. Gidopoulos, and N. N. Lathiotakis, [J. Chem. Phys. 136 , 224109 \(2012\)](#).
12. "Nonanalyticity of the optimized effective potential with finite basis sets", N. I. Gidopoulos, and N. N. Lathiotakis, [Phys. Rev. A 85, 052508 \(2012\)](#).