Natalia E. KOVAL, PhD

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RESEARCH INTERESTS

- Ion-matter interaction: dynamics, electronic and plasmon excitations
- Electronic stopping processes in materials and biological matter
- Defect formation in materials under irradiation

SKILLS

- **Methods:** Density functional theory (DFT). Time-dependent density functional theory (TDDFT). *Ab initio* molecular (Born-Openheimer) dynamics (AIMD). Ehrenfest dynamics. Linear response TDDFT. Classical MD.
- **Computational techniques/codes:** Electronic structure, density of states, elastic properties (SIESTA & VASP & CP2K codes). TDDFT, Ehrenfest dynamics, and AIMD (SIESTA & CP2K & Qb@ll codes). Evolutionary structure search (USPEX code). Other codes include: MBPT-LCAO, YAMBO, LAMMPS.
- **Programming/data analysis:** Python, Matplotlib, Panda, SciPy, machine learning with Scikit-learn, LaTeX, Gnuplot, Fortran, Linux, MacOS, Shell.
- **Languages:** Russian (native), English (professional working proficiency), Spanish (professional working proficiency), French (limited working proficiency).
- **Soft skills:** analytical, problem solver, fast learner, independent, open minded, collaborative, meeting deadlines, focused and organised.

EXPERIENCE

- **1.04.2023 – current**: **Postdoctoral Researcher**
  Materials Physics Center, San Sebastián, Spain.
- **15.11.2022 – 31.01.2023**: **Visiting researcher**
  Instituto de Fusión Nuclear "Guillermo Velarde", Universidad Plitécnica de Madrid, Madrid, Spain
- **01.12.2018 – 30.06.2022**: **Postdoctoral researcher**
  CIC Nanogune BRTA, San Sebastián, Spain
- **01.06.2016 – 31.11.2018**: **Postdoctoral researcher**
  Materials Physics Center MPC (CFM), University of the Basque Country UPV/EHU, and Donostia International Physics Center (DIPC), San Sebastián, Spain.

EDUCATION

- **2016**: **PhD in Physics** from the University of the Basque Country UPV/EHU.

  Thesis title: Electron dynamics in the interaction of atomic particles with spherical metal clusters.
  Supervisors: Dr. Ricardo Díez Muiño, Dr. Daniel Sanchez-Portal.
  PhD thesis defense: April 22, 2016, highest mark (*Cum laude*).

- **2011**: **Master in Nanoscience** from Materials Physics Department, University of the Basque Country (Universdidad del Pais Vasco - UPV/EHU), San Sebastian, Spain.

  Master thesis: Energy loss of electrons photoemitted from metal clusters.
  Supervisors: Dr. Ricardo Díez Muiño, Dr. Daniel Sánchez-Portal.

- **2007**: **University degree in Physics** from Department of Physics, Adyghe State University, Maykop, Russia.
  Major: Computational methods in physics. Diploma *Summa cum laude*.

  Diploma project: High harmonic generation in atoms: strong field approximation for TDDFT.
  Diploma project advisors: Prof. Tlyachev Vyacheslav Beslanovich, Dr. Peter Koval.

RESEARCH LINE

– Starting at Adyghe State University (ASU, Maykop, Russia), I am continuously working with density functional theory (DFT) and time-dependent DFT. My diploma project at ASU was devoted to the development of a quantum model of a high-harmonic generation in atoms and its application for simple atoms, such as H and He. More precisely, I developed a code applying TDDFT in the strong field approximation to calculate the spectrum of radiation of a model helium atom placed in a strong laser field. As a result, I have shown that there is a second plateau in the spectrum of He due to a double recombination following a non-sequential ionization.

– During my PhD study at the University of the Basque Country, I used real-time TDDFT to study energy loss and dynamic screening processes for ins and molecules interacting with metal clusters. The most relevant result of my PhD project is the first *ab initio* calculation of the electronic stopping power ratio for hydrogen ions interacting with silicon dioxide and carbon, which has shown excellent agreement with experimental results.

– As a postdoctoral researcher at CFM/MPC (Donostia-San Sebastián, Spain), I studied the structure and properties of high-entropy alloys (HEAs). I used evolutionary algorithms implemented in the USPEX code to predict the crystal structure of complex multicomponent alloys. I used DFT (VASP code) to calculate the electronic and elastic properties of HEAs with the aim of understanding how the chemical composition and the electronic structure of the alloys affect their elastic properties. Three articles, in two of which I am the first author, were published as a results of this work. One article has been featured on the cover of the Journal of Applied Physics.

– As a postdoctoral researcher in the theory group at CIC Nanogune (Donostia-San Sebastián, Spain), I participated in the ESC2RAD project. I studied space radiation effects on solar cells using real-time TDDFT and AIMD within the SIESTA and CP2K codes. I focused on radiation effects on solar cells and on biological matter. In particular, I studied the electron scattering in water by means of linear response theory (LR-TDDFT) related to biological damage. Moreover, I managed four HPC projects with the leading role in the writing of grant proposals. We were awarded 48 million core-hours of the HPC time on national (Barcelona, Spain) and international (Paris, France, within the PRACE project) computational facilities.

  I have also been involved in the QSENSE project (QUANTUM SENSE. Molecular Scale Probe for Sensing Quantum Spins). I performed DFT calculations to study electronic and magnetic properties of molecules and nanostructures in collaboration with the experimental group.

  Currently, I am working on different aspects of ion-matter and light matter interactions in the context of catalysis. In particular, I study effects of plasmon excitation on catalytic activity of metal nanoparticles. I also apply neural networks to study ion-matter interaction.

PUBLICATIONS

Peer-reviewed Articles

2023 Manuel Vilas-Varela, Francisco Romero-Lara, Alessio Vegliante, Jan Patrick Calupitan, Adrián Martínez,[a] Lorenz Meyer, Unai Uriarte-Amiano, Niklas Friedrich, Dongfei Wang, Fabian Schulz, Natalia E. Koval, María E. Sandoval- Salinas, David Casanova, Martina Corso, Emilio Artacho, Diego Peña, José Ignacio Pascual, *On-Surface Synthesis and Characterization of a High-Spin Aza-[5]-Triangulene*, Angewandte Chemie (2023) e202307884.

2023 Natalia E. Koval, Fabiana Da Pieve, Bin Gu, Daniel Muñoz-Santiburcio, Jorge Kohanoff, and Emilio Artacho, *Nonlinear electronic stopping of negatively-charged particles in liquid water*, Phys. Rev. Research 5 (2023) 033063.

2023 Johannes L. Teunissen, Thomas Jarrin, Nicolas Richard, Natalia E. Koval, Daniel Muñoz Santiburcio, Jorge Kohanoff, Emilio Artacho, Fabrizio Cleri, and Fabiana Da Pieve, *Effect of electronic stopping in molecular dynamics simulations of collision cascades in gallium arsenide*, Phys. Rev. Materials 7 (2023) 025404.

2022 Natalia E. Koval, Daniel Sánchez-Portal, Andrei G. Borisov, and Ricardo Díez Muiño, *Time-dependent density functional theory calculations of electronic friction in non-homogeneous media*, Phys. Chem. Chem. Phys. 24 (2022) 20239-20248.

2022 Natalia E Koval, Peter Koval, Fabiana Da Pieve, Jorge Kohanoff, Emilio Artacho, Dimitris Emfietzoglou, *Inelastic scattering of electrons in water from first principles: cross sections and inelastic mean free path for use in Monte Carlo track-structure simulations of biological damage*, R. Soc. Open Sci. 9, 212011 (2022) 212011.

2020 F. Da Pieve, G. Gronoff, J. Guo, C. J. Mertens, L. Neary, B. Gu, N. E. Koval, J. Kohanoff, A. C. Vandaele, F. Cleri, *Radiation Environment and Doses on Mars at Oxia Planum and Mawrth Vallis: Support for Exploration at Sites With High Biosignature Preservation Potential*, Journal of Geophysical Research: Planets 125, e2020JE006488.

2020 Natalia E. Koval, Fabiana Da Pieve, Emilio Artacho, *Ab initio electronic stopping power for protons in $Ga_{0.5}In_{0.5}P/GaAs/Ge$ triple-junction solar cells for space applications*, R. Soc. Open Sci. 7 (2020) 200925.

2020 Natalia E. Koval, Joseba Iñaki Juaristi, Ricardo Díez Muiño, and Maite Alducin, *Structure and properties of CoCrFeNiX multi-principal element alloys from ab initio calculations*, J. Appl. Phys. 127 (2020) 145102.

2019 F. Matias, P. L. Grande, M. Vos, Peter Koval, Natalia E. Koval, and N. R. Arista, *Nonlinear stopping effects of slow ions in a no-free-electron system: Titanium nitride*, Phys. Rev. A 100, (2019) 030701(R).

2019 Natalia E Koval, Joseba Iñaki Juaristi, Ricardo Díez Muiño, Maite Alducin, *Elastic properties of the TiZrNbTaMo multi-principal element alloy studied from first principles*, Intermetallics 106 (2019) 130-140.

2018 Flávio Matias da Silva, Raul Carlos Fadanelli Filho, Pedro Luis Grande, Nestor Arista, Natalia Koval, Gregor Schiwietz, *Stopping power of cluster ions in a free-electron gas from partial-wave analysis*, Phys. Rev. A 98 (2018) 062716.

2018 Jon Mikel Sanchez, Iban Vicario, Joseba Albizuri, Teresa Guraya, Natalia E. Koval and Jose Carlos Garcia, *Compound formation and microstructure of as-cast high entropy aluminums*, Metals 8 (2018) 167.

2017 F. Matias, R. C. Fadanelli, P. L. Grande, N. E. Koval, R. Díez Muiño, A. G. Borisov, N. R. Arista and G. Schiwietz, *Ground- and excited-state scattering potentials for the stopping of protons in an electron gas*, J. Phys. B: At. Mol. Opt. Phys. 50 (2017) 185201 (8pp).

2017 N. E. Koval, A. G. Borisov, L. F. S. Rosa, E. Stori, J. F. Dias, P. L. Grande, D. Sánchez-Portal, and R. Díez Muiño, *Vicinage effect in the energy loss of H_2 dimers: Experiment and calculations based on time-dependent density functional theory*, Phys. Rev. A 95, 062707 (2017).

2013 N. E. Koval, D. Sánchez-Portal, A. G. Borisov, and R. Díez Muiño, *Dynamic screening and energy loss of antiprotons colliding with excited Al clusters*, Nucl. Instr. Meth. B 317 (2013) 56–60, http://dx.doi.org/10.1016/j.nimb.2013.01.053. Proceeding of the 19th International Workshop on Inelastic Ion- Surface Collisions (IISC-19).

2012 N. E. Koval, D. Sánchez-Portal, A. G. Borisov, and R. Díez Muiño, *Dynamic screening of a localized hole during photoemission from a metal cluster*, Nanoscale Res. Lett. 7:447 2012.

2009 P. G. Koval, N. E. Koval, D. Foerster, *On the theory of electronic excitation in molecules on the basis of Petersilka-Gossmann-Gross equation*, The Bulletin of the Adyghe State University, Issue 2(49), – 2009 (in Russian).

Book Chapters

3. Natalia E. Koval, Bin Gu, Daniel Muñoz-Santiburcio and Fabiana Da Pieve, *Modeling Radiation Damage in Materials Relevant for Exploration and Settlement on the Moon*, In **Lunar Science - Habitat and Humans** edited by Dr. Yann Chemin, InTechOpen, 2022, DOI: 10.5772/intechopen.102808.

2. Apostolova, Tzveta; Artacho, Emilio; Cleri, Fabrizio; Cotelo, Manuel; Crespillo, Miguel L.; Da Pieve, Fabiana; Dimitriou, Vasilis; Djurabekova, Flyura; Duffy, Dorothy M.; García, Gastón; García-Lechuga, Mario; Gu, Bin; Jarrin, Thomas; Kaselouris, Evaggelos; Kohanoff, Jorge; Koundourakis, George; **Koval, Natalia**; Lipp, Vladimir; Martin-Samos, Layla; Medvedev, Nikita; Molina-Sánchez, Alejandro; Muñoz-Santiburcio, Daniel; Murphy, Samuel T.; Nordlund, Kai; Oliva, Eduardo; Olivares, José; Papadogiannis, Nektarios A.; Redondo-Cubero, Andrés; Rivera de Mena, Antonio; Sand, Andrea E.; Sangalli, Davide; Siegel, Jan; Solov'yov, Andrey V.; Solov'yov, Ilia A.; Teunissen, Johannes; Vázquez, Elisa; Verkhovtsev, Alexey V.; Viñals, Sílvia y Ynsa, María Dolores (2021). **Tools for investigating electronic excitation: experiment and**

multi-scale modelling. Instituto de Fusión Nuclear "Guillermo Velarde", Universidad Politécnica de Madrid. ISBN 978-84-09-36032-1. `https://doi.org/10.20868/UPM.book.69109`.

1. I. D. Andrievskiy, N. E. Koval, V. B. Tlyachev. Selected questions of the theory of multiphoton ionization and high-harmonic generation. – Scientific-methodical edition for students studying physics. Maykop, Adyghe State University, Russia. (In Russian)

REVIEWER

Peer-reviewer for: Nano Letters; Materials Letters; Materials Science in Semiconductor Processing; Solar Energy Materials and Solar Cells; Journal of Alloys and Compounds; Physical Chemistry Chemical Physics; Vacuum.

STUDENT SUPERVISION

2021-2022 **Nuria Santervás Arranz**, master thesis at UPV/EHU and CIC Nanogune: Electronic friction between two graphene layers. Co-supervised together with Emilio Artacho.

2021-2022 **Unai Uriarte**, graduate student final year project (successfully defended on May 10, 2022, with the mark 9 out of 10): Electronic properties of low-dimensional carbon structures with density functional theory. Co-supervised together with Emilio Artacho.

2021 **Mónica Tapia Del Moral**, summer internship student at CIC Nanogune. Project: Real-time TDDFT calculations of the electronic stopping power for electrons in liquid water.

2019 **Ainhoa Smithers**, summer internship student at CIC Nanogune. Co-supervised together with Emilio Artacho. Project: Testing real-time TDDFT implementation in the SIESTA code.

GRANTS

– HPC PRACE grant of 31,40 M core hours on Joliot Curie - SKL cluster for a period of 12 months awarded to the Theory group at CIC Nanogune.

– Trainee grant of 975 euro from the COST Action CA17126 to participate in the 1st TUMIEE Training School "Training young researchers on multidisciplinary approaches to electronic excitation problems", 23/09 to 4/10/2019.

INTERNATIONAL CONFERENCES and SHOOLS

24. *Rethinking ab initio plasmonic photocatalysis: a comparative analysis of previous findings*, poster presentation at the NANOP – Nanophotonics and Micro/Nano Optics International Conference, Barcelona, Spain, November 27 – 29, 2023.

23. *Inelastic scattering of electrons in liquid water: energy loss function and cross-sections from time-dependent density functional theory*, poster presentation at the COSIRES 2022, The 15th conference of COmputer Simulation of IRradiation Effects in Solids, Porquerolles, France, May 22 – 26, 2022.

22. *Low-energy electron projectiles in water: Linear vs non-linear energy loss*, N. Koval, F. Da Pieve, B. Gu, J Kohanoff, E. Artacho, presented by Emilio Artacho at the APS March Meeting 2022, Chicago, March 14 – 18, 2022.

21. *Inelastic scattering of protons and electrons by liquid water: a time-dependent density-functional theory approach to radiation damage*, **Invited talk** at the Meeting of the COST Action TUMIEE "Towards Understanding and Modelling Intense Electronic Excitation" (CA17126), Aix-Marseille University (France), September 30 – October 1, 2021.

20. Liverpool Inorganic Crystal Structure Prediction Tools, Online Workshop, April 13, 2021, The University of Liverpool.

19. *Radiation-induced effects in solar cells for future space missions: a combined Monte Carlo and ab-initio study of proton impact, electronic stopping and threshold displacement energy*, F. Da Pieve, N. E. Koval, D. Muñoz-Santiburcio, J. Teunissen, and E. Artacho, presentation by F. Da Pieve at the APS March Meeting 2021, March 15–19, 2021; Virtual; Time Zone: Central Daylight Time, USA.

18. *Recent Advancements in the Modelling of radiation effects on Solar Cells for future missions to Mars*, D. Muñoz-Santiburcio, N. E. Koval, J. Teunissen, E. Artacho, F. Da Pieve, presentation by F. Da Pieve at The 8th Annual IEEE International Conference on Wireless for Space and Extreme Environments (WISEE 2020), October 12 to 14, 2020, Virtual conference.

17. *Electronic Stopping Power for Protons in Solar-Cell Materials from First-Principles Calculations*, poster presentation at the "Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (MiniTotalEnergy2020)", San Sebastián, Spain, January 8 – 10, 2020.

16. Participated in the 1st TUMIEE Training School "Training young researchers on multidisciplinary approaches to electronic excitation problems", Hellenic Mediterranean University, Crete, Greece, September 23 - October 4, 2019.

15. *Electronic Stopping Power for Protons in Solar-Cell Materials from First-Principles Calculations*, poster + flash presentation (5 minutes) at the 26th International Symposium on Ion-Atom Collisions (ISIAC), Paris, France, July 20–22, 2019.

14. *Ab initio calculations of structure and elastic properties of light-weight HEAs*, poster presentation at the 2018 TMS Annual Meeting & Exhibition, Phoenix, AZ, USA, March 11–15, 2018. Symposium: High Entropy Alloys VI.

13. *Ab initio calculations of structure and elastic properties of light-weight HEAs*, poster presentation at the APS March Meeting 2018, Los Angeles, CA, USA, March 5 – 9, 2018.

12. *Ab initio Calculations of the Structure and Elastic Properties of Low-Weight High Entropy Alloys*, poster presentation at EUROMAT 2017, European congress and exhibition on advanced materials and processes, Thessaloniki, Greece, September 17 – 22, 2017. Symposium D8: Ab initio models for thermodynamic and elastic properties of advanced materials.

11. Software Carpentry Workshop, Materials Physics Center - University of the Basque Country, 28–30 June 2017, San Sebastián - Donostia, Spain. Version control with Git, Programming with Python, Introduction to Scientific Python. http://iamc.eu/2017-06-28-cfmehu/

10. *TDDFT calculations of the electronic friction for antiprotons colliding with metal clusters.* **Invited talk**: at the workshop "Theoretical Chemistry and Physics at the Quantum Scale", Symposium Bordeaux-Euskampus, "Week 26", Bordeaux, France, June 26, 2017.

9. *Vicinage effect in the energy loss of a hydrogen dimer from TDDFT calculations.* **Invited talk**: at the VIII Taller de Colisiones Inelásticas en la Materia, Playa del Carmen, Quintana Roo, México, December 11–14, 2016.

8. International Symposium on Material Design & the 11^{th} USPEX Workshop, Varenna, Lake Como, Italy, June 5–9, 2016.

7. *Vicinage effect in the energy loss of hydrogen dimer from TDDFT simulations.* Oral contribution at the 21^{st} International Workshop on Inelastic Ion-Surface Collisions (IISC-21), organized by Donostia International Physics Center, Donostia-San Sebastián, Spain, October 18–23, 2015.

6. *Dynamic screening and charge transfer processes in photoemission from an adsorbate on a metal cluster.* Poster presentation at the Psi-k 2015 Conference, San Sebastián, Spain, September 6–10, 2015.

5. *Dynamic screening and charge transfer processes in photoemission from an adsorbate on a metal cluster.* Poster presentation at the CECAM Workshop on the Perspectives of the many-particle methods: total energy, spectroscopy and time-dependent dynamics, Bremen, Germany, April 20–24, 2015.

4. *Vicinage effect in the energy loss of antiprotons in metals from TDDFT simulations.* Oral contribution at the 26^{th} International Conference on Atomic Collisions in Solids (ICACS-26), Debrecen, Hungary, July 13–18, 2014.

3. *Energy loss and charge transfer processes during photoemission from metal clusters and adsorbates.* Oral contribution at the 30^{th} Brandt Ritchie Workshop (BRW), Passion for Knowledge - Quantum 13, Donostia International Physics Center (DIPC), Donostia - San Sebastián, Spain, October 1–4, 2013.

2. *Dynamic screening of a localized hole and a photoelectron emitted from a metal cluster.* Oral contribution at the 19^{th} International Workshop on Inelastic Ion-Surface Collisions (IISC-19), organized by Max-Planck-Institut für Plasmaphysik, Frauenchiemsee, Germany, September 16–21, 2012.

1. *Dynamic screening of a localized hole during photoemission from a metal cluster.* Poster presentation at the International CAMD′12 Summer School "Electronic Structure Theory and Materials Design", at the Technical University of Denmark, August 11–17, 2012.