

## Ana S. Dobrota

### Research field/areas

- Materials modelling
- DFT calculations
- Surface functionalization
- Electrochemical energy conversion and storage systems
- Graphene based materials

### Education

- 2014 – 2017: Ph.D. in Physical Chemistry (Physical Chemistry of Materials, Quantum Chemistry, Electrochemistry), Faculty of Physical Chemistry, University of Belgrade, Serbia. Average grade: 10. Thesis title: *Theoretical analysis of graphene functionalization for energy conversion and storage applications*. Defended: 25.12.2017. Supervisor: Dr. Igor Pašti, associate professor.
- 2013 – 2014: M.Sc. in Electrochemistry and Chemical Kinetics, Faculty of Physical Chemistry, University of Belgrade, Serbia. Average grade: 10. Final paper: *Theoretical analysis of H, O and OH adsorption on grapheme-oxide*. Defended: 17.07.2014. Supervisor: Dr. Igor Pašti, assistant professor.
- 2009 – 2013: B.Sc. in Physical Chemistry, Faculty of Physical Chemistry, University of Belgrade, Serbia. Average grade: 9.89. Final paper: *Theoretical study of Ni<sub>x</sub>Mo<sub>1-x</sub> surfaces*. Defended: 15.07.2013. Supervisor: Dr. Igor Pašti, assistant professor.

### Employment history

- 2016 – present: *Teaching Assistant*, Faculty of Physical Chemistry, University of Belgrade, Serbia.
- 2016 – 2017: *Part-time Teaching Assistant*, Faculty of Agriculture, University of Belgrade, Serbia.
- 2015 – 2016: *Research Trainee*, Faculty of Physical Chemistry, University of Belgrade, Serbia.

### List of selected publications

1. A.S. Dobrota, I.A. Pašti, S.V. Mentus, B. Johansson, N.V. Skorodumova. Functionalized graphene for sodium battery applications: the DFT insights. *Electrochim. Acta* 250 (2017): 185–195 (ISSN 0013-4686, Impact Factor 5.116, Category M21) <https://doi.org/10.1016/j.electacta.2017.07.186>
2. A.S. Dobrota, I.A. Pašti, S.V. Mentus, N.V. Skorodumova. A DFT study of the interplay between dopants and oxygen functional groups over the graphene basal plane – implications in energy-related applications. *Phys. Chem. Chem. Phys.* 19(12) (2017): 8530-8540 (ISSN 1463-9076, Impact Factor 3.906, Category M22) <https://doi.org/10.1039/C7CP00344G>
3. A.S. Dobrota, I.A. Pašti, S.V. Mentus, N.V. Skorodumova. A general view on the reactivity of the oxygen-functionalized graphene basal plane. *Phys. Chem. Chem. Phys.* 18(9) (2016) 6580-6586 (ISSN 1463-9076, Impact Factor 4.123, Category M21) <https://doi.org/10.1039/C5CP07612A>
4. D. Chanda, J. Hnát, A.S. Dobrota, I.A. Pašti, M. Paidar, K. Bouzek. The effect of surface modification by reduced graphene oxide on the electrocatalytic activity of nickel towards the hydrogen evolution reaction. *Phys. Chem. Chem. Phys.* 17(40) (2015) 26864-26874 (ISSN 1463-9076, Impact Factor 4.449, Category M21) <https://doi.org/10.1039/C5CP04238K>
5. A.S. Dobrota, I.A. Pašti, N.V. Skorodumova. Oxidized graphene as an electrode material for rechargeable metal-ion batteries—a DFT point of view. *Electrochim. Acta* 176 (2015) 1092-1099 (ISSN 0013-4686, Impact Factor 4.803, Category M21) <https://doi.org/10.1016/j.electacta.2015.07.125>

### Citations

- According to SCOPUS, her publications have been cited 173 times. The total citation number of her publications has reached 210 according to Google Scholar.
- Her Hirsch index is 8 in SCOPUS and 10 in Google Scholar.

### Project history

She has participated in 1 national and several international projects:

- 2015 – present: *Lithium ion batteries and fuel cells – research and development*, Ministry of Education, Science and Technological Development of the Republic of Serbia (III45014) (participant).
- 2015 – present: *Modelling of Complex Materials*, Swedish National Infrastructure for Computing (participant).
- 2019 – 2020: *New approaches to the understanding of the electrochemical properties of nanocarbons under operating conditions*, Ministry of Education, Science and Technological Development of the Republic of Serbia and Deutcher Akademischer Austauschdienst DAAD (participant).
- 2018 – 2019: *Fundamental insights into fuel cell electrocatalysis - combination of modelling and experiment*, Ministry of Education, Science and Technological Development of the Republic of Serbia and Slovenian Research Agency ARRS (participant).

- 2018 – 2019: *Theoretical and experimental development of novel sensor based on graphene composites for the detection of organophosphate pesticides*, Ministry of Education, Science and Technological Development of the Republic of Serbia and Deutcher Akademischer Austauschdienst DAAD (participant).
- 2015 – 2018: *DURAPEM - Novel materials for durable proton exchange membrane fuel cells*, NATO Emerging Security Challenges Division, SPS Programme (participant).
- 2017 – 2018: *Conducting polymer composites*, DANUBE REGION project (participant).

#### Awards

- *Sestre Bulajić foundation* award for the best B.Sc. thesis.
- *Pupin award of Matica srpska* for the best M.Sc. thesis.

#### Reviewing

She reviewed for the following journals:

- *Journal of Materials Chemistry A* (1 paper; ISSN 2050-7488, Impact Factor 10.733, Category M21a)
- *Applied Surface Science* (1 paper; ISSN 0169-4332, Impact Factor 5.155, Category M21)
- *International Journal of Hydrogen Energy* (2 papers; ISSN 0360-3199, Impact Factor 4.084, Category M22).

#### International scientific collaboration and mobility

- Study visit to Multiscale Materials Modeling Group, KTH Royal Institute of Technology, Stockholm, Sweden (November/December 2015.).
- Guest researcher at PDC-KTH *Center for High Performance Computing*, Stockholm, Sweden, through *HPC-Europa3 H2020 programme “Transnational Access Programme for a Pan-European Network of HPC Research Infrastructures and Laboratories for scientific computing”* (June/July 2018).

#### Other professional activities

- TRAIN (Training & Research for Academic Newcomers) certificate.
- Organizing committee member for the conferences 2<sup>nd</sup> and 3<sup>rd</sup> *International Meeting on Materials Science for Energy Related Applications* (2016 and 2018.) and local executive committee member for conferences *Physical Chemistry 2016* and *Physical Chemistry 2018*.
- Technical Editor of the Book of Abstracts for the conference 3<sup>rd</sup> *International Meeting on Materials Science for Energy Related Applications* (2018., Belgrade, Serbia).
- Volunteer for Science promoting activities.
- Member of the Society of Physical Chemists of Serbia.

#### Links

ORCID profile: <https://orcid.org/0000-0001-6200-8612>

SCOPUS profile: <https://www.scopus.com/authid/detail.uri?authorId=56769958200>

Google Scholar profile: <https://scholar.google.com/citations?user=4PPjLsAAAAJ&hl=en&oi=ao>

ResearchGate profile: [https://www.researchgate.net/profile/Ana\\_Dobrota](https://www.researchgate.net/profile/Ana_Dobrota)