

Curriculum Vitae

Milena Petković

Born: 10.06.1976

Education:

- BSc (2000), Faculty of Physical Chemistry, University of Belgrade
- PhD (2004), Institut für Chemie, Freie Universität, Berlin, Germany

Work experience:

- 2000 - research and teaching assistant, Faculty of Physical Chemistry, University of Belgrade
- 2001-2004. scientific coworker, Institut für Chemie, Freie Universität, Berlin, Germany
- 2005 - research and teaching assistant, Faculty of Physical Chemistry, University of Belgrade
- 2007 - Assistant Professor, Faculty of Physical Chemistry, University of Belgrade
- 2014 - Associate Professor, Faculty of Physical Chemistry, University of Belgrade
- 2019 - Full Professor, Faculty of Physical Chemistry, University of Belgrade

Teaching:

As a research and teaching assistant at Faculty of Physical Chemistry, University of Belgrade:

- Exercises in *Quantum chemistry and molecular structures* for undergraduate students, Faculty of Physical Chemistry, University of Belgrade
- Exercises in *General and physical chemistry* for undergraduate students, Faculty of Biology, University of Belgrade
- Exercises in *Physical Chemistry 1* for undergraduate students, Faculty of Chemistry, University of Belgrade
- Exercises in *Physical Chemistry 2* for undergraduate students, Faculty of Chemistry, University of Belgrade
- Exercises in *Chemical kinetics* for undergraduate students, Faculty of Physical Chemistry, University of Belgrade

As a scientific coworker at Freie Universität, Berlin:

- Exercises in *Quantum chemistry* for undergraduate students
- Exercises in *Quantum chemistry on the computer 1*, International Bilingual Master Program in Chemistry
- Exercises in *Quantum chemistry on the computer 2*, International Bilingual Master Program in Chemistry
- Exercises in *Kinetics on the computer with introduction to UNIX and Fortran* for undergraduate students

As an Assistant Professor, Associate Professor and Full Professor at Faculty of Physical Chemistry, University of Belgrade:

- Teaching undergraduate course *General course in physical chemistry 2*, Faculty of Physical Chemistry, University of Belgrade
- Teaching undergraduate course *Physical chemistry of fluids*, Faculty of Physical Chemistry, University of Belgrade
- Teaching undergraduate course *Physical Chemistry I*, Faculty of Chemistry, University of Belgrade
- Teaching master's level course *Modelling processes in the environment*, Faculty of Physical Chemistry, University of Belgrade
- Teaching master's level course *Selected Chapters of Environmental Physical Chemistry*, Faculty of Physical Chemistry, University of Belgrade
- Teaching master's level course *Methods and Methodologies in Contemporary Physical Chemistry Research*, Faculty of Physical Chemistry, University of Belgrade
- Teaching graduate course *New Physico-chemical Methods*

Books:

1. *Applied Quantum Chemistry* (in Serbian), M. Petković, Faculty of Physical Chemistry, University of Belgrade, 2013
2. *Physical Chemistry of Fluids* (in Serbian), M. Petković, Faculty of Physical Chemistry, University of Belgrade, 2017

Publications:

1. *Multidimensional hydrogen bond dynamics in salicylaldehyde: Coherent nuclear wave packet motion versus intramolecular vibrational energy redistribution*, M. Petković, O. Kühn, *J. Phys. Chem. A* 107 (2003) 8458-8466
<http://pubs.acs.org/doi/abs/10.1021/jp035688r>
2. *Ultrafast wave packet dynamics of an intramolecular hydrogen transfer system: From vibrational motion to reaction control*, M. Petković, O. Kühn, *Chem. Phys.* 304 (2004) 91-102
<http://www.sciencedirect.com/science/article/pii/S0301010404002794>
3. *Cascaded energy redistribution upon O-H stretching excitation in an intramolecular hydrogen bond*, K. Heyne, E.T.J. Nibbering, T. Elsaesser, M. Petković, O. Kühn, *J. Phys. Chem. A* 108 (2004) 6083-6086
<http://pubs.acs.org/doi/abs/10.1021/jp048653f>
4. *Multidimensional quantum dynamics and infrared spectroscopy of hydrogen bonds*, K. Giese, M. Petković, H. Naundorf, O. Kühn, *Phys. Rep.* 430 (2006) 211-276
<http://www.sciencedirect.com/science/article/pii/S0370157306001608>
5. *Infrared spectroscopy of ClONO₂ and BrONO₂ investigated by means of anharmonic force fields*, M. Petković, *Chem. Phys.* 331 (2007) 438-446
<http://www.sciencedirect.com/science/article/pii/S030101040600615X>

6. *Are the program packages for molecular structure calculations really black boxes?*, A. Mraković, M. Drvendžija, A. Samolov, M. Petković, M. Perić, *J. Serb. Chem. Soc.* 72 (2007) 1329-1341
http://www.shd.org.rs/JSCS/Vol72/No12/JSCS_V72_No12-17.pdf
7. *Renner-Teller effect in five-atomic molecules: Ab initio investigation of the spectrum of C₅⁻*, M. Perić, M. Petković, S. Jerosimić, *Chem. Phys.* 343 (2008) 141-157
<http://www.sciencedirect.com/science/article/pii/S0301010407003060>
8. *Proton and protonic entities in solid heteropoly compounds: An ab initio calculation of the environmental effect on the H₅O₂⁺ ion*, U.B. Mioč, M. Petković, M. Davidović, M. Perić, T. Abdul-Redah, *J. Mol. Struct.* 885 (2008) 131-138
<http://www.sciencedirect.com/science/article/pii/S0022286007006862>
9. *Shaping the infrared spectrum of the acetic acid dimer in the OH-stretching range: Multiple conformers and anharmonic coupling*, M. Petković, J. Novak, N. Došlić, *Chem. Phys. Lett.* 474 (2009) 248-252
<http://www.sciencedirect.com/science/article/pii/S0009261409004436>
10. *IR spectrum of the O-H...O hydrogen bond of phthalic acid monomethylester in gas phase and in CCl₄ solution*, Y.-a. Yan, M. Petković, G.M. Krishnan, O. Kühn, *J. Mol. Struct.* 972 (2010) 68-74
<http://www.sciencedirect.com/science/article/pii/S0022286009007935>
11. *Vibrational spectroscopy: Can density functional theory cope with highly electronegative atoms?*, M. Petković, *Spec. Acta - Part A* 77 (2010) 942-947
<http://www.sciencedirect.com/science/article/pii/S1386142510004142>
12. *Localization of the counterion of the protonated schiff base of n-butylretinal in solution*, N. Biliškov, J. Novak, M. Petković, G. Zgrablić, G. Baranović, N. Došlić, *Cro. Chem. Acta* 84 (2011) 221-231
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13. *O-H stretch in phenol and its hydrogen-bonded complexes: Band position and relaxation pathways*, M. Petković, *J. Phys. Chem. A* 116 (2012) 364-371
<http://pubs.acs.org/doi/abs/10.1021/jp209897y>
14. *Quantum-chemical investigation of the photoproduct of the reaction of two 1-methylthymine molecules: The pyrimidine(6-4)pyrimidone adduct*, M.M. Ristić, M. Petković, M. Etinski, *J. Serb. Chem. Soc.* 77 (2012) 1037-1045
<https://pdfs.semanticscholar.org/3a95/5094f8d474b512cb96d5f8961969a2dff94b.pdf>
15. *Study on vibrational relaxation dynamics of phenol-water complex by picosecond time-resolved IR-UV pump-probe spectroscopy in a supersonic molecular beam*, Y. Miyazaki, Y. Inokuchi, T. Ebata, M. Petković, *Chem. Phys.* 419 (2013) 205-211
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16. *Proučavanje strukture i vibracionih svojstava ciklobutan pirimidin dimera | [Investigation of structure and vibrational properties of cyclobutane pyrimidine dimer]*, M.M. Petković, M.R. Etinski, M.M. Ristić, *Hem. ind.* 67 (2013) 203-207
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17. *Vibrational spectroscopy of picolinamide and water: From dimers to condensed phase*, V. Jovanović, Y. Miyazaki, T. Ebata, M. Petković, *J. Phys. Chem. A* 117 (2013) 6474-6482
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18. *A study of the low-lying singlet and triplet electronic states of chlorophyll a and b*, M. Etinski, M. Petković, M.M. Ristić, *J. Serb. Chem. Soc.* 78 (2013) 1775-1787
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19. *In vitro anti-hydroxyl radical activity of the fructooligosaccharides 1-kestose and nystose using spectroscopic and computational approaches*, B. Pejin, A. G. Savić, M. Petković, K. Radotić, M. Mojović, *Int. J. Food. Sci. Tech.* 49 (2014) 1500-1505
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20. *Intramolecular OHO bonding in dibenzoylmethane: symmetry and spectral manifestations*, M. Petković, M. Etinski, *RSC Advances*. 4 (2014) 38517-38526
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21. *Extending the chemistry of carbonates: P-N bond cleavage via an S_N2' -line mechanism*, C. Gurnani, N. Đorđević, S. Muthaiah, D. Dimić, R. Ganguly, M. Petković, D. Vidović, *Chem. Comm.* 53 (2015) 10762-10764
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22. *Electron-vibrational coupling and fluorescence spectra of tetra-, penta- and hexacoordinated chlorophylls c_1 and c_2* , M. Etinski, M. Petković, M. M. Ristić, C. M. Marian, *J. Phys. Chem. B* 119 (2015) 10156-10169
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23. *Oxidation of a P-C bond under mild conditions*, D. Vidović, G. Ilić, R. Ganguly, M. Petković, *Chem. Eur. J.* 21 (2015) 18594-18597
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24. *Control of a photoswitching chelator by metal ions: DFT NBO and QTAIM analysis*, D. Dimić, M. Petković, *Int. J. Quant. Chem.* 116 (2016) 27-34
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26. *Stability and Anharmonic N-H Stretching Frequencies of 1-Methylthymine Dimers: Hydrogen Bonding Versus π -Stacking*, M. Petković, M. M. Ristić, M. Etinski, *J. Phys. Chem. A* 120 (2016) 1536-1544
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27. *Bis(carbodicarbene)phosphenium trication: the case against hypervalency*, Nemanja Đorđević, Rakesh Ganguly, Milena Petković, Dragoslav Vidović, *Chem. Comm.* 52 (2016) 9789-9792
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28. *A new insight into photochemistry of avobenzene in gas phase and acetonitrile from ab initio calculations*, M. Kojić, M. Petković, M. Etinski, *Phys. Chem. Chem. Phys.* 18 (2016) 22168-22178

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32. *Alkene-assisted cis-to-trans isomerization of non-conjugated polyunsaturated alkenes*, A. V. Smarun, F. Duzhin, M. Petković, D. Vidović, *Dalton. Trans.* 46 (2017) 14244-14250

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33. *Site-specific deuteration of polyunsaturated alkenes*, A. V. Smarun, M. Petković, Mikhail S. Shchepinov D. Vidović, *J. Org. Chem.* 82 (2017) 13115-13120

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34. *E-H (E = B, Si, C) Bond Activation by Tuning Structural and Electronic Properties of Phosphenium Cations*, N. Đorđević, R. Ganguly, M. Petković, D. Vidović, *Inorg. Chem.* 56 (2017) 14671-14681

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35. *Mechanistic insights on how hydroquinone disarms OH and OOH radicals*, Đ. Nakarada, M. Petković, *Int. J. Quantum. Chem.* 118 (2018) e25496

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36. *New insight into Uracil Stacking in Water from Ab ignition Molecular Dynamics*, B. Milovanović, M. Kojić, M. Petković, M. Etinski, *J. Chem. Theo. Comp.* 14 (2018) 2621-2632

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37. *When hydroquinone meets methoxy radical: Hydrogen abstraction reaction from the viewpoint of interacting quantum atoms*, M. Petković, Đ. Nakarada, M. Etinski, *J. Comp. Chem.* 39 (2018) 1868-1877

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38. *Tuning the electronic and chemisorption properties of hexagonal MgO nanotubes by doping – Theoretical study*, A. Jovanović, M. Petković, I. A. Pašti, B. Johansson, N. V. Skorodumova, *Appl. Surf. Sci.* 457 (2018) 1158-1166

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39. *Raman spectra of aqueous uracil stacked dimer: first principle molecular dynamics simulation*, B. Milovanović, M. Petković, M. Etinski, *Chem. Phys. Lett.* 713 (2018) 15-20

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40. *New hybrid cluster-continuum model for pKa values calculations: Case study of neurotransmitters' amino group acidity*, M. M. Ristić, M. Petković, B. Milovanović, J. Belić, M.

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41. *Theoretical scrutinization of nine benzoic acid dimers: Stability and energy decomposition analysis*, I. Petrović, B. Milovanović, M. Etinski, M. Petković, *Int. J. Quantum Chem.* (2019) e25918
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42. *A simulation of free radicals induced oxidation of dopamine in aqueous solution*, B. Milovanović, J. Ilić, I. M. Stanković, M. Popara, M. Petković, M. Etinski, *Chem. Phys.* 524 (2019) 26-30
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43. *Hydrogen transfer reaction: Bond formation and bond cleavage through the eyes of Interacting Quantum Atoms*, B. Ž. Milovanović, M. R. Etinski, M. M. Petković, *J. Serb. Chem. Soc.* 84 (2019) 891-900
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44. *Elucidating Solvent Effects on Strong Intramolecular Hydrogen Bond: DFT-MD Study of Dibenzoylmethane in Methanol Solution*, B. Milovanović, Ivana Stanković, M. Petković, M. Etinski, *ChemPhysChem* (2019)
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