List of Publications – Sept 2014
Oana Cramariuc

A. Peer-reviewed scientific articles in Journals

1. E. Vuorimaa, T. Vuorinen, N. Tkachenko, O. Cramariuc, T. Hukka, S. Nummelin, A. Shivanyuk, K. Rissanen, H. Lemmetyinen: Photoinduced electron transfer between a self-assembled resorcinarene – [60]fullerene complex and poly(3-hexylthiophene) in Langmuir – Blodgett films. Langmuir 17, 2001, 7327 – 7331.
2. O. Cramariuc, T. I. Hukka, T. T. Rantala: A DFT study of asymmetric meso-substituted porphyrins and their zinc complexes. Chem. Phys. 305, 2004, 13 – 26.
3. O. Cramariuc, T. I. Hukka, T. T. Rantala: Time-dependent Density Functional Calculations on the Electronic Absorption Spectra of an Asymmetric *meso*-substituted Porphyrin and its Zinc Complex. J. Phys. Chem. A, 108, 2004, 9441.
4. Kirsi Tappura, O. Cramariuc, T. I. Hukka, T. Rantala: Molecular Simulations for the Conformational Assessment of a Porphyrin – Fullerene dyad in different environments. Phys. Chem. Chem. Phys., 7, 2005, 3126.
5. O. Cramariuc, T. I. Hukka, T. T. Rantala, and H. Lemmetyinen, A TD-DFT description of photoabsorption and electron transfer in a covalently bonded porphyrin-fullerene dyad. J. Phys. Chem. A, 110, 2006, 12470.
6. K. Tappura, O. Cramariuc, T. L .J. Toivonen, T. I. Hukka and T. T. Rantala, Computational analysis of the conformations of a doubly linked porphyrin-fullerene dyad. Chem. Phys. Lett., 424, 2006, 156.
7. T. L. J. Toivonen, T. I. Hukka, O. Cramariuc, T. T. Rantala and H. Lemmetyinen: DFT and TDDFT Study Related to Electron Transfer in Nonbonded Porphine...C60 Complexes, J. Phys. Chem. A 110, 2006, 12213.
8. O. Cramariuc, T. I. Hukka, T. T. Rantala, and H. Lemmetyinen, A theoretical study of the electronic structure and excited states of a doubly-linked porphyrin-fullerene dyad. J. Comp. Chem., http://dx.doi.org/10.1002/jcc.21143, 2008.
9. M. Vasilescu, R. Bandula, O. Cramariuc, H. Lemmetyinen, T. Hukka, F. Dumitrascu. Optical Spectroscopic Characteristics and TD-DFT Calculations of new Pyrrolo[1,2-b]-pyridazines Solutions. Journal of Photochemistry and Photobiology, A: Chemistry (2008), 194(2-3), 308-317; ***award by the Romanian National Council for Research and Education.***
10. Viitala, M.; Cramariuc, O.; Rantala, T. T.; Golovanov, V. Small hydrocarbon adsorbates on SnO2(110) surfaces. Density functional theory study. Surface Science (2008), 602(18), 3038-3042.
11. P. J. Aittala, O. Cramariuc, M. Vasilescu, R. Bandulea, T. I. Hukka, Effect of Substituents on the Absorption Properties of Three Pyridylindolizine Derivatives: A DFT and TDDFT study. Chemical Physics 2009, 360, 162-170.
12. P. J. Aittala, O. Cramariuc, T. I. Hukka, M. Vasilescu, R. Bandula, H. Lemmetyinen, A TDDFT study of the fluorescence properties of three alkoxypyridylindolizine derivative, J Phys Chem A. 2010 Jul 8;114(26):7094-101.

13. P. Aittala, O. Cramariuc, T. I. Hukka, Electric-Field-Assisted Electron Transfer in a Porphine−Quinone Complex: A Theoretical Study, J. Chem. Theory Comput., 2010, 6 (3), pp 805–816.
14. V. Golovanov, M. Viitala, T. Kortelainen, O. Cramariuc, T.T. Rantala, Stability of siloxane couplers on pure and fluorine doped SnO_2 (110) surface: A first principles study, Surface Science 604 (2010) 1784–1790.
15. B. Cramariuc, O. Cramariuc, A brief review of HPC provided as a web service by SMEs - present situation and future trends, J. Appl. Comp. Sci. & Math., 7 – Special Issue 2010.
16. M. Viitala, O. Cramariuc, B. Delly, T. T. Rantala, Conformation and energetics of benzene adsorbate on SnO_2 (110) surfaces: A first principles study, Surface Science, Surface Science, 605 (15–16), 2011, 1563–1567.
17. Polishchuk, A. V.; Karaseva, E. T.; Emelina, T. B.; Cramariuc, O. & Karasev, V. E. Spectral-luminescent properties and molecular orbital treatment of some mono- and difluoroquinolones. J Fluoresc, 2011, 21, 1293-1300.
18. P. Aittala, O. Cramariuc, T. I. Hukka, The Excited States of a Porphine–Quinone Complex under an External Electrostatic Field Calculated by TDDFT, Chem. Phys. Lett., 2011, 501(4-6), 226-231.
19. A. V. Polishchuk, E. T. Karaseva, T. B. Emelina, O. Cramariuc and Vladimir E. Karasev, Polymorphism and Intramolecular Proton Transfer in Fluoroquinolone Compounds, J. Fluoresc., doi: 10.1007/s10895-011-0912-5.
20. E. S. Lohan, A. Rusu-Casandra, O. Cramariuc, I. Marghescu, B. Cramariuc, End-User Attitudes towards Location-Based Services and Future Mobile Wireless Devices: The Students' Perspective, Information 2011, 2(3), 426-454.
21. A.V. Polischuk, T.B. Emelina, O. Cramariuc, V.I. Chukharev, E.T. Karaseva, V.E. Karasev, Photolysis and quantum mechanical calculations of nalidixic acid radical states, Russian Journal of General Chemistry, 02/2012; 82(2):323-328. DOI:10.1002/chem.201103843 pp.323-328.
22. A.V.Polischuk, E.T. Karaseva, O. Cramariuc, V.E. Karasev. New fluoroquinolone-based luminophores activators. Russian Journal of General Chemistry, 344-346, 2011 (in Russian).
23. B. Cramariuc, R. Cramariuc, R. Scarlet, L. R. Manea, I. G. Lupu, O. Cramariuc, Fiber diameter in electrospinning process, J. Electrostatics, 71(3), 2013, 189–198.
24. O. Cramariuc, T. Rog, I. Vattulainen, Drug-Lipid Membrane Interaction Mechanisms Revealed through Molecular Simulations, ***Invited review article*** to Current Physical Chemistry, vol. 2, 379-400 (2012).
25. O. Cramariuc, T. Rog, L. Monticelli, A. V. Polishchuk, I. Vattulainen, Mechanism for translocation of fluoroquinolones across lipid membranes, BBA-Biomembranes, Biochimica et Biophysica Acta – Biomembranes, 1818 (11), 2012, 2563–2571. ranked in the ***top 20 articles*** of the journal for almost one year after its publication.
26. O Cramariuc, P. Aittala, T.I. Hukka, Molecular dipole effects on tuning electron transfer in a porphine-quinone complex: a DFT and TDDFT study. Journal of Molecular Modeling, 2013, 19: (2): 697-704.
27. S. Pöyry, O. Cramariuc, P. A. Postilaa, K. Kaszuba, M. Sarewiczb, A. Osyczkab, I. Vattulainen, T. Róg, Atomistic simulations indicate cardiolipin to have an

integral role in the structure of the cytochrome bc1 complex, Biochimica et Biophysica Acta (BBA) – Bioenergetics, 1827(6), 2013, 769–778.

28. K. Kaszuba, P. A. Postila, O. Cramariuc, M. Sarewicz, A. Osyczka, I. Vattulainen, T. Róg, Parameterization of the prosthetic redox centers of the bacterial cytochrome bc 1 complex for atomistic molecular dynamics simulations, accepted for publications, Theoretical Chemistry Accounts, April 2013, 132:1370.
29. L. YC, S. Rissanen, M. Stepniewski, O. Cramariu, T. Róg, S. Mirza, H. Xhaard, M. Wytrwal, M. Kepczynski, A. Bunker, Study of interaction between PEG carrier and three relevant drug molecules: piroxicam, paclitaxel, and hematoporphyrin, J Phys Chem B. 2012 Jun 21;116(24):7334-41.
30. I. G. Lupu, O. Cramariuc, H. I. Hogas, L. Hristiana, Parameters optimization for the production of needle-punched nonwoven agrotextiles, 2013, Journal of The Textile Institute, DOI: 10.1080/00405000.2013.777581.
31. A. Polishchuk, T. Emelina, E. Karaseva, O. Cramariuc, V. Chukharev, V. Karasev, Photochemical Behavior and Photolysis of Protonated Forms of Levofloxacin, Photochem. Photobio. (2014), 90, 79-84.
32. M. Niskanen, M. Kuisma, O. Cramariuc, V. Golovanov, T. I. Hukka, N. Tkachenko, T. T. Rantala, Porphyrin adsorbed on the (1011) surface of the wurtzite structure of ZnO - conformation induced effects on the electron transfer characteristic, Phys. Chem. Chem. Phys., 2013, DOI: 10.1039/C3CP51685G.
33. S. Poyry, O. Cramariuc, P. Postila, K. Kaszuba, M. Sarewicz, A. Osyczka, T. Rog, I. Vattulainen, Clarifying the Roles of Cardiolipin, Biophys. J., 2014, 1006, 513A.
34. P. Postila, O. Cramariuc, S. Poyry, K. Kaszuba, I. Vattulainen, M. Sarewicz, A. Osyczka, T. Rog, Bridging a Gap Between Cytochrome Bc1 Complex Structure and Function. Biophys. J., 2014, 1006, 586A.
35. A. Maciejewski, M. Pasenkiewicz-Gierula, O. Cramariuc, I. Vattulainen, T. Rog, Refined OPLS All-Atom Force Field for Saturated Phosphatidylcholine Bilayers at Full Hydration. J. Phys. Chem. B (2014), 118, 4571-4581.
36. T. Karilainen, O. Cramariuc, M. Kuisma, K. Tappura, T. Hukka. Van der Waals interactions are critical in Car-Parrinello molecular dynamics simulations of porphyrin-fullerene dyads. Second revision for J. Comp. Chem.
37. M. Lehto, T. Karilainen, T. Róg, O. Cramariuc, E. Vanhala, J. Tornaeus, H. Taberman, J. Jänis, H. Alenius, I. Vattulainen, O. Laine, Occupational Health Hazard of Co-Exposure to Fullerene and Organic Industrial Chemicals Estimated by in Vitro Toxicological and Molecular Modeling Studies, Second revision for PLOS ONE.

B. Full peer-review articles in international scientific compilation works and international scientific conference proceedings with a referee practice

1. Polishchuk A.V., Karaseva E.T., Cramariuc O., Karasev V.E. New luminofor-activators based on (fluoro)quinolone antibacterials, Institute of Chemistry FEB RAS, ISIF, 01-06 September 2008, Vladivostok, Russia.

2. O. Cramariuc, J. Ojanen, K. Tappura, T. Hukka, T.T. Rantala, TDDFT Calculations on Photoabsorption of Porphyrin-Fullerene dyads, ***invited paper***, AIP Conference Proceedings, ICCMSE 2008.
3. E. S. Lohan, O. Cramariuc, A. Rusu-Casandra, I. Marghescu, B. Cramariuc, User requirements in the context of future location based services as seen from a survey among romanian students, In Proc. Int. Conf. on Localization and GNSS, June 29-30, pg, 19 – 24, 2011, Tampere, Finland.
4. O. Cramariuc, B. Cramariuc, Approaches to Linking Biomolecular Simulations and Computational Systems Biology, In Proc. Int. Workshop Genom. Sig. Proc., 26-29 June, 2011, Bucharest, Romania. **Invited paper**
5. C. Ramassamy, V. Ricordel, O. Cramariuc, B. Cramariuc, Lattice Vector Quantization for the Analysis of Molecular Data, In Proc. of Sign. Proc. Appl. Math. Electronics and Comm., pg. 97-100, 26-28 Aug., 2011, Cluj-Napoca, Romania.

C. Scientific monographs

1. O. Cramariuc: Strategies of modeling cyclic organic molecules using molecular mechanics, semiempirical and ab initio methods with applications to calix[4]arene and its derivatives, Master Thesis, Tampere University of Technology, Institute of Materials Chemistry, 2001

2. O. Cramariuc, Computational Characterization of Photoabsorption and Structure of Porphyrin-Fullerene Dyads, PhD thesis, Tampere University of Technology, Tampere, Finland, 2006.

D. Books/Book chapters

1. B. Cramariuc, L. Nisiparu, O. Cramariuc, Nano-electrotechnologies: theoretical aspects, in "Theoretical Fundaments of Electrospinning (in Romanian), Editors B. Cramariuc, L. R. Manea, I. G. Lupu, Ed. Iaşi: Tehnopress, 2009, ISBN 978-973-702-581-4.

E. Other scientific publications

1. Oana Cramariuc, Terttu Hukka, Tapio Rantala: Density functional calculations on the optical absorption spectrum of a porphyrin derivative. Finnish Symposium on Quantum Chemistry. An International Conference in Honor of Professor Pekka Pyykkö. June 11 – 17, 2001. Kuusamo, Finland.

2. E. Vuorimaa, T. Vuorinen, N. Tkachenko, O. Cramariuc, T. Hukka, K. Rissanen, H. Lemmetyinen: Photoinduced electron transfer between a self-assembled resorcinarene – [60]fullerene complex and poly(3-hexylthiophene) in Langmuir – Blodgett films. ICP XX International Conference on Photochemistry. July 30 – August 4, 2001. Moscow, Russia.

3. Oana Cramariuc, Terttu Hukka, Tapio Rantala: Density functional calculations on the optical absorption spectrum of a porphyrin and its zinc derivative. Proceedings of the XXXVI Annual Conference of the Finnish Physical Society. March 14 – 16, 2002. Joensuu, Finland. p. 291.

4. Oana Cramariuc, Terttu Hukka, Tapio Rantala: Density functional calculations on the optical absorption spectrum of a substituted porphyrin and its zinc complex. Fourth Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV). July 9 – 16, 2002. INJEP, Marly-le-Roi, France.

5. Oana Cramariuc, Terttu Hukka, Tapio Rantala: Optical absorption spectra of a substituted porphyrin and its zinc complex. Cecam Psi-k Workshop, Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials. September 23 – 26, 2002. CECAM, Ecole Normal Superieure de Lyon, France.

6. Oana Cramariuc, Terttu Hukka, Tapio Rantala: Comparative DFT/TD-DFT study on electronic structures and optical absorptions of porphyrins and their zinc complexes. Proceedings of the XXXVII Annual Conference of the Finnish Physical Society. March 20 – 22, 2003. Helsinki, Finland. p. 324.

7. O. Cramariuc, T. Hukka, T. Rantala: Time-dependent density functional calculations on the electronic absorption spectra of an asymmetric meso-substituted porphyrin and its zinc complex. Proceedings of the XXXVIII Annual Conference of the Finnish Physical Society. March 18 – 20, 2004. Oulu, Finland. p. 121.

8. K. Tappura, O. Cramariuc, T. I. Hukka, and T. T. Rantala: A dft/td-dft study of a porphyrin-fullerene dyad and its Consituent electron-donor molecule. Winter School in Theoretical Chemistry, December 13 – 16, 2004. Helsinki, Finland.

9. K. Tappura, O. Cramariuc, T. I. Hukka, and T. T. Rantala: Simulations of solvent and temperature effects on a porphyrine-fullerene dyad. Proceedings of the XXXIX Annual Conference of the Finnish Physical Society. March 17 – 19, 2005. Espoo, Finland. p. 193.

10. K. Tappura, O. Cramariuc, T. I. Hukka, T. L. J. Toivonen and T. T. Rantala: Molecular simulations of a doubly linked porphyrin-fullerene dyad. Submitted to the XXXIX Annual Conference of the Finnish Physical Society. March 9 – 11, 2006. Tampere, Finland.

11. Oana Cramariuc, Terttu Hukka, Tapio Rantala: A theoretical study of the electronic structure and excited states of a linked porphyrin-fullerne dyad. XXXVII Annual Conference of the Finnish Physical Society. March 9 – 11, 2006. Tampere, Finland.

12. O. Cramariuc, K. Tappura, T.I. Hukka, H. Lemmetyinen, and T. T. Rantala, Molecular dynamics simulations and quantum mechanical calculations of a doubly linked porphyrin-fullerene dyad IVC-17/ICSS-13 and ICN+T2007, Stockholm 2-6 July, 2007.

13. P. Aittala, O. Cramariuc, T. I. Hukka, T. T. Rantala, M. Vasilescu, R. Bandula, F. Dumitrascu, Substitution and solvent effects on the optical properties of new pyridylindolizine derivatives: a theoretical study, Conference on Computational Physics, 5-8 Brussel, 2007.

14. M. Viitala, O. Cramariuc, T. T. Rantala, First-principles study of molecular adsorption on SnO_2 surfaces, Conference on Computational Physics, 5-8 Brussel, 2007.

15. M. Viitala, O. Cramariuc, T. T. Rantala, V. Golovanov, Small hydrocarbon adsorbates on SnO_2 surfaces, Accepted at the Annual Conference of the Finnish Physical Society. April 2008, Turku, Finland.

16. O. Cramariuc, A. Polishchuk, V. Karasev, I. Vattulainen, T. T. Rantala, E. Karaseva, Structure and Medium Effects on the Photophysical Behavior of Ciprofloxacine, 11-12 December, 2008, Ab initio modeling in applied Biosciences, Uppsala, Sweden.

17. B. Cramariuc, O. Cramariuc, T. I. Hukka, A conformational search and clustering algorithm of cyclic molecules, In Proc. ICQC-2009, pp. 370, Helsinki, Finland

18. O. Cramariuc, I. Vattulainen, A better PSMF for transcription binding site prediction, Linking Systems Biology and Biomolecular Simulations, CECAM-HQ-EPFL, Lausanne, Switzerland, November 16, 2009.

19. O. Cramariuc, J. Iglesias-Fernández, K. Kaszuba, T. Rog, Carme Rovira and I. Vattulainen, A computational QM/MM insight on the iron-sulfur cluster in cytocrhome bc1, Physics Days 2013, March 14th - 16th 2013 Dipoli, Espoo, Finland.