

Studies

Physical Faculty, Moscow State University "M.V. Lomonosov", Moscow, Russia, 1984-1990

Ph.D. in Physics and Mathematics of the Physical Faculty, Moscow State University "M.V. Lomonosov", Moscow, Russia, 1990-1993 (Solid State Physics, Molecular Dynamics Simulation of condensed matter)

Post-doc in INFM, unita Modena, Modena, Italy, 2001

Research projects

"Car-Parrinello Molecular Dynamics", Physics department, University of Rome "La Sapienza", in collaboration with Cambridge University and CASPUR, 2003-2005

"Non-linear dynamical systems and quantum and classical molecular dynamics", Physics department, University of Rome "La Sapienza", 2002-2003

"Molecular dynamics of proteins in solutions", INFM and Physics department of the Modena and Reggio Emilia University, 2001 (during post-doc, directed by M. Ferrario). During this project added the molecular pressure calculation and the molecular NPT propagator to the program DLPROTEIN.

Publication list

1. "The inelastic hard dimer gas: a non-spherical model for granular matter", G. Constantini, U. Marini Bettolo, G. Kalibaeva, G. Ciccotti, J. Stat. Phys. (2005) in press

<http://adsabs.harvard.edu/abs/2004cond.mat.11747C>

2. "Molecular dynamics of complex systems: non-Hamiltonian, constrained, quantum-classical", G. Ciccotti and G. Kalibaeva, Contribution into the book "Novel methods in soft matter simulation" by Mikko Karttunen, Ilpo Vattulainen and Ari Lukkarinen, Springer Verlag (2004)

<http://www.springerlink.com/index/QQFLAUQU5YWPE5G.pdf>

3. "Deterministic and stochastic algorithms for mechanical systems under constraints", G. Ciccotti and G. Kalibaeva, Phil. Trans. R. Soc. Lond. A, 362, p. 1583 (2004)

<http://www.ingentaconnect.com/content/rsi/rta/2004/00000362/00001821/art00004;jsessionid=1qv7jf86slgab.victoria>

4. "Simulation of diatomic liquids using hard spheres model", G. Ciccotti and G. Kalibaeva, J. Stat. Phys., 115, p. 701 (2004)

<http://www.kluweronline.com/article.asp?PIPS=479124&PDF=1>

5. "Constant pressure – constant temperature molecular dynamics: a correct constrained NPT ensemble using the molecular virial", G. Kalibaeva, M. Ferrario, G. Ciccotti, Mol. Physics, 101, p. 765 (2003)

<http://taylorandfrancis.metapress.com/app/home/contribution.asp?wasp=d08999fqlpcuwv8f9w9h&referrer=parent&backto=issue,6,16;journal,39,191;linkingpublicationresults,1:100678,1>

6. "X ray study and structure simulation of the amorphous tungsten oxide", L.A. Lugovskaya, L.A. Aleshina, G.M. Kalibaeva, A.D. Fofanov, Acta Cryst., B58, p. 576 (2002)

<http://journals.iucr.org/b/issues/2002/04/00/av0052/index.html>

7. "Problem-based learning: Analysis of advantages and disadvantages of its applications in the classroom in light of a problem solving approach and project-oriented method", F. C. Perez, G. Kalibaeva, Revista Mexicana De Psicología 18, N1, p. 80 (2001)

<http://www.unimaas.nl/pbl/Publications/Pa-Pz.htm>

8. "Microstructure of Ni-P alloys and Its Effect on Resistivity", V.S. Stepanyuk, A.A. Katsnelson, A. Szasz, G. Kalibaeva, A. Hendry, Physica Status Solidi (b) 176, K63 (1993)

9. "Long range oscillating interaction potentials and stable structures", O.V. Volf, G.M. Kalibaeva, V.S. Stepanyuk, A.A. Katsnelson, Vestnik MGU, serie "Física y Astronomía", v.34, N2 (1993) (in Russian)

10. "Effect of impurity mass on the microstructure of rapidly quenched aluminium", V.S. Stepanyuk, A. Szasz, A.A. Katsnelson, O.V. Wolf, E. Gyarmati, G.M. Kalibaeva, Journal of Physics: Condensed Matter, 5, N34, p. 6139-6148 (1993)

http://adsabs.harvard.edu/cgi-bin/nph-bib_query?bibcode=1993JPCM....5.6139S&db_key=PHY

11. "Effects of isolated perturbations on the microstructure of amorphous metals", O.V. Volf, G.M. Kalibaeva, V.S. Stepanyuk, A.A. Katsnelson, Fizica Tviordogo Tela, 35, p.385-388, 1993 (in Russian) translated into English by "American Institute of Physics": Sov. Phys. Solid State, 35(2), p.197-198 (1993)

12. "Concentrational dependence of Al-Mn alloys", V.S. Stepanyuk, A.A. Katsnelson, A. Szasz, G.M. Kalibaeva, H.Muller and H.Kirchmayr, Physica Status Solidi (b) 178, K1 (1993)

13. "Short-range order in dilute Ni-P and Ni-B alloys", G.M. Kalibaeva, S.A.Gromov, V.S. Stepanyuk, A.Szasz, A.A.Katsnelson, Fizica Tviordogo Tela, 34, p.3597 (1992) (in Russian); Translated into English by "American Institute of Physics": Sov. Phys. Solid State, 34(11), p.1926-1927, 1993

14. "Characteristics of the icosahedral microstructure of the Al_{77.5}Mn_{22.5} alloy", V.S. Stepanyuk, G.M.Kalibaeva, A.A. Katsnelson, Fizica Tviordogo Tela, 34, p.1194 (1992) (in Russian); Translated into English by "American Institute of Physics": Sov. Phys. Solid State, 34(4), p.632-634, 1992

15. "Nature of Mooij correlation in Ni-P alloys", V.S. Stepanyuk, A.A. Katsnelson, G.M.Kalibaeva, A. Szasz, Fizica Tviordogo Tela, 33, p. 3095 (1991) (in Russian); Translated into English by "American Institute of Physics": Sov. Phys. Solid State , 33(10), p. 1749-1950, 1992

Useful links

<http://www.cpmid.org/>

<http://www.sissa.it/cm/DLPROTEIN/>

http://www.sissa.it/cm/DLPROTEIN/user_guide.html

<http://www.cecarn.fr/>

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