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Appendix I to the Edital nº 224/2016

THE VICE-RECTOR OF FUNDAÇÃO UNIVERSIDADE FEDERAL DO ABC (UFABC), appointed by Portaria UFABC nº 98, dated February 11th 2014, published in Diário Oficial da União (DOU), Section 2, page 15, date February 13th 2014, exercising the power conferred upon him makes public, through the current Appendix, the Program Content, Suggested Bibliography and further information pertaining to the Edital nº 224/2016, from 30/08/2016, published in Section 3 from DOU nº 168, dated 31/08/2016, page 50:

1. Appendix I to the Edital 224/2016 - Field: Physics; Sub-field: Computational Material Science

1.1. Program content:
1.1.1. Written exam: The Drude theory and Sommerfeld for the electron gas. Crystal lattices: structures, classification and determination. Reciprocal lattices. Electronic band structure. Fermi surface. Semiconductors. Magnetism. Molecular Orbital theory. Hartree-Fock method. Density Functional Theory. Classical and ab initio molecular dynamics. Atomistic empiricial models for materials

1.1.2. Lecture exam: Experimental motivations of Quantum Mechanics. Quantization. Uncertainty relations. Time-dependent and time-independent Schrodinger equation. Reflection, Transmission and tunneling. Schrodinger equation in spherical coordinates. Hydrogen atom. Angular momentum and spin. Schrodinger equation for 2-body and many body systems. Atoms and periodic table. Fundamental and excited states: spectra of atoms, diatomic and polyatomic molecules. Molecular interactions. Crystal lattices. Electronic bands.

1.2. – Suggested Bibliography:
1.2.1. Written exam
1.2.1.1. Charles Kittel, Introduction to Solid State Physics, Wiley.

1.2.1.2. Neil W. Ashcroft and N. David Mermin, Solid State Physics, Cengage Learning.

1.2.1.3. Daan Frenkel e Berend Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2 ed., 2001.

1.2.1.4. Donald A McQuarrie, Simon; John D. Simon, Physical chemistry: a molecular approach. University Science Books, 1997.

1.2.1.5. Frederick Reif, Fundamentals of Statistical and Thermal Physics, Waveland Press Inc, 2008.

1.2.1.6. M. P. Allen, D. J. Tildesley , Computer simulation of liquids, Clarendon Press, 1987

1.2.1.7 Richard M. Martin, Electronic Structure: Basic Theory and Practical Methods, Cambridge University Press, 2008.

1.2.2. Lecture exam
1.2.2.1. D. Halliday, R. Resnick, J.Walker, Fundamentals of Physics.

1.2.2.2. R. A. Serway, J. W. Jewett Jr., Principles of Physics.

1.2.2.3. H. Moysés Nussenzveig, Curso de Física Básica, Editora Edgard Blücher Ltda.

1.2.2.4. R. B. Leighton, M. Sands, R. P. Feynman, The Feynman Lectures on Physics, Addison-Wesley.

1.2.2.5. P. A. Tipler, R. A. Llewellyn, Modern Physics.

1.2.2.6. P. Atkins, Physical-Chemistry.

2. For the selection process, in addition to what is specified by the Edital UFABC de Condições Gerais nº 96/2013, candidates must be productive and up-to-date to the international state of the art subjects in computational materials science. The position is open to candidates with a wide variety of profiles, ranging from applied simulations to the development of methodologies and theories for the study of atomic and molecular systems, liquids and solids at a fundamental level. Candidates with demonstrated experience in the study of systems in atomic level and/or macroscopic systems are welcome.

3. And, to make it public to the interested potential candidates, ISSUE the current Appendix.

Santo André, November 23rd 2016.

Dácio Roberto Matheus
Vice-Reitor