212050 – ADVANCED STATISTICAL THERMODYNAMICS APPLIED TO SOLIDS AND INTERFACES

CREDITS: 04 (four) – 60 hours/class

CONTENT:

Construction of the specific expressions of partition functions and thermodynamic potentials for solids and gases. Simulations of thermodynamic potentials for molecular adsorption and reactive chemisorption. Eyring's Theory: fundamentals and practical applications. Addition of solvent effect to thermodynamic problems of adsorption and reaction. Classical dynamics applied to intercalation compounds and molecular diffusion in solids. Fundamentals and applications of the Grand-Canonical Monte Carlo technique.

SYLLABUS:

1. Review of statistical thermodynamics concepts;
2. Thermodynamic potentials for solids and gases;
3. Thermodynamics of adsorption and reactions between gases and solids;
4. Solvent effect and ion exchange processes;
5. Phase diagrams T x mole fraction and other phase diagrams;
6. High pressure processes, phase transformations;
7. Thermodynamics of high pressure reactions;
8. Fundamentals of classical mechanics and classical dynamics;
9. Classical dynamics applied to interspersed lamellar compounds;
10. Classical dynamics applied to nanoporous compounds;
11. Fundamentals of classic Monte Carlo simulation;
12. Application of the Gran-Canonical Monte Carlo methodology in the accumulation of gases in materials.

BIBLIOGRAPHY:

1. ATKINS, P.; DE PAULA, J. Físico-Química. 8ª Edição. Rio de Janeiro: LTC, 2008. Vol. 1. 592 págs. (ISBN: 8521616007).
2. SIMON, J. D.; MCQUARRIE, D. A. Physical Chemistry. Mill Valey, CA, USA: University Science Books, 1998. 1360 págs. (ISBN: 0935702997).
3. Recent scientific articles.
4. Manuals of the codes used.