Questions for diploma exam – NT II

InterMath: Joint double degree Msc programme
Mathematics for new materials design

1. The molecular dynamics (MD) method: principle of operation, advantages and limitations.
2. Periodic boundary conditions in computer simulations. Physical meaning and applicability, main limitations.
3. Empirical potentials. Physical meaning, applications, limitations.
4. Statistical interpretation of the wave function.
5. Operators in quantum mechanics. Meaning, mathematical structure and properties.
6. Time-dependent Schrödinger equation. Formulation and solving methods.
7. Variational Ritz method. Description and applicability.
8. Triplet and singlet open-shell states of molecules. General description, energy of states (which state has lower energy and why).
9. Estimation of energy of a chemical reaction for which the spins of the reactants and product are different.
10. Comparison of sputtering and evaporation PVD processes.
11. Determination of chemical composition. List and describe briefly at least 3 methods.
12. Dynamical Systems: Linearization around an equilibrium point.
13. Hamiltonian Systems.
14. Structural Stability.
15. Hilbert spaces.
16. Bounded linear operators on Banach spaces.
17. Spectrum and resolvent of bounded linear operators on Hilbert spaces.
18. Transient and permanent response specifications for feedback control systems.
19. Finite-time response of digital control systems.
20. Controllability, observability and the separation principle.
21. Definition of characteristic vectors and characteristic surfaces for linear partial differential operators.
22. Classification of second order linear PDEs.
23. Fundamental solution for heat equation and Laplace equation.
24. D'Alembert formula.

Dziekan

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