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Quantum-chemical methods in the theory of heterogeneous catalysis

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Abstract

In the survey there has been given the formal systematization of quantum-chemical calculation models. Emphasis is made on three methods which have been used in computations of chemical adsorption and catalysis. Description of calculation models ranging from semi-empirical MO LCAO to post-hartri-fock calculations have been presented. Theory of DFT, applicability of different calculation models to cluster approach have been discussed in detail, solid state (zone) computation methods have been described.