Simulation of chemical bonds formation during adsorption

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The article describes main mathematical approaches to the description of interatomic interactions: quantum-mechanical methods, molecular dynamics methods based on empirical potentials and molecular dynamics methods based on approximation of tight-binding. Merits and demerits of the considered approaches are given. Theoretical part presents the mathematical apparatus for approximate calculation of the wave equation of the atom on the basis of the Hamiltonian and the theory of tight-binding. A correcting algorithm of calculation of kinematic characteristics is used for modeling movements of the interacting atoms. The authors consider two methodological stages: settlement on which initial conditions are set and levels of energy barriers of possible chemical reactions, and model stage where the assessment of forces of interatomic interaction is made are defined. A specific feature of modeling is in combination of the methods of molecular dynamics with approximation of tight-binding. The advantage of such approach is in significant increase of the size of the system without considerable loss of calculation accuracy. The methodology is demonstrated by an example of chemical bonds formation at adsorption.

Keywords: *computer simulation, molecular dynamics methods, tight-binding approximation, heterogeneous systems*

REFERENCES

[1] Paine M.C., Teter M.P., Allan D.C., Arias T.A., Joannopoulos J.D. Iterative Minimization Techniques for ab initio Total-Energy Calculations: Molecular Dynamics and Conjugate Gradients. *Rev. Modern Phys*., 1992, vol. 64, pp. 1045–1097.

[2] Patrice E.A., Gonis A., Colombo L. *Tight-Binding Approach to Computational Materials Science*. Boston, MIT, 1998, 542 p.

[3] Tersoff J. Empirical Interatomic Potential for Carbon, with Applications to Amorphous Carbon. *Phys. Rev. Lett*., 1988, vol. 61, pp. 2879–2882.

[4] Tersoff J. Modeling Solid-State Chemistry: Interatomic Potentials for Multicomponent Systems. *Phys. Rev. B*, 1989, vol. 39, pp. 5565–5568.

[5] Brenner D.W. Empirical Potential for Hydrocarbons for Use in Simulating the Chemical Vapor Deposition of Diamond Films. *Phys. Rev. B*, 1990, vol. 42, pp. 9458–9471.

[6] Brenner D.W., Shenderova O.A., Harrison J.A., Stuart S.J., Ni B., Sinnott S.B. A Second-Generation Reactive Empirical Bond Order (REBO) Potential Energy Expression for Hydrocarbons. *J. Phys. Condens. Matter*, 2002, vol. 14, pp. 783–802.

[7] Wang C.Z., Ho K.M. Tight-Binding Molecular Dynamics Studies of Covalent Systems. *Adv. Chem. Phys*., 1996, vol. XCIII, pp. 651–702.

[8] Wang C.Z., Ho K.M. Environment Dependent Tight-Binding Potential Model. *Phys. Rev. B*, 1996, vol. 53, pp. 979–987.

[9] Wang C.Z., Ho K.M. Material Simulations with Tight-Binding Molecular Dynamics. *J. Phase Equil*., 1997, vol. 18, pp. 516–527.

[10] Liu Z.P., Hu P. General Rules for Predicting where a Catalytic Reaction should Occur on Metal Surfaces. *J. Am. Chem. Soc*., 2003, vol. 125, pp. 1958–1967.
[11] Verlet L. Computer Experiments on Classical Fluids. *Phys. Rev*., 1968, vol. 159, pp. 98–103.
[12] Ivanov V.A., Rabinovich A.P., Khokhlov A.R. *Metody kompyuternogo modelirovaniya* [Computer simulation methods]. Moscow, Librokom, 2009, 662 p.
[13] Berendsen H.J.C., Postma J.P.M., Gunsteren W.F., Dinola A., Haak J.R. Molecular Dynamics with Coupling to an External Bath. *J. Chem. Phys*., 1984. vol. 81, pp. 3684–3690.
[14] Xu C.H., Wang C.Z., Chan C.T., Ho K.M. A Transferable Tight-Binding Potential for Carbon. *J. Phys. Condens. Matter*, 1992, vol. 4, pp. 6047–6054.
[15] Li X.P., Nunes R.W., Vanderbilt D. Density-matrix Electronic-structure Method with Linear System-Size Scaling. *Phys. Rev. B*, 1993, vol. 47, pp. 10891–10894.

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