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Technique of Definition Areas Requiring a Quantum Description Within of the Hybrid Method (Quantum Mechanics / Molecular Mechanics)

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The new model, which determines the active area (the region for which high-precision quantum methods must be used) of the structure,was developed within the of the hybrid method (QM/MM). Problem of determining atoms with the critical tension values is the basis of this model. The potential energy of these atoms and its nearest neighbours was calculated by quantum-chemical method. The potential energy of the rest structure was calculated by molecular mechanical method. The Hybrid method (QM/MM) allows to reveal with high accuracy optimum topology structure and increase the speed of finding its equilibrium state.

Key words: the quantum-chemical methods, the molecular mechanics methods, the critical tension values, the force, the carbon nanostructures.

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