Zastosowanie metod dynamiki molekularnej w badaniach nad układami z wiązaniami wodorowymi = An application of molecular dynamics methods in investigations of systems with hydrogen bonds.

Autorzy

Aneta Jezierska

Jarosław Panek

Rok wydania

2017

Czasopismo

Wiadomości Chemiczne

Numer woluminu

71

Strony

473-495

Kolekcja

Naukowa

Język

Polski

Typ publikacji

Artykuł

Streszczenie

Modern computational chemistry offers a wide variety of methods allowing us to investigate very complex systems. In the current study, we would like to focus on ab initio and classical molecular dynamics to show their applications in our rese-arch. Car-Parrinello molecular dynamics (CPMD) was carried out to study com-pounds possessing intra- and intermolecular hydrogen bonds. Our simulations were performed in vacuum, in solvent and in crystalline phase. It is well known that intramolecular hydrogen bonding stabilizes 3D structure of molecules. The strength of the bonding and its features are influenced by inductive and steric effects. Our short overview on CPMD application to systems with intramolecular HB we start from Schiff and Mannich bases -model compounds to investigate intramolecular hydrogen bonding. Other examples reported here derive from the class of N-oxide type compounds. Special attention was devoted to another representative structure in such investigations – picolinic acid N-oxide. In some examples listed above pro-ton transfer phenomena occurred making these compounds interesting objects for future excited state studies. Aliphatic boronic acid was used as a model example to study intermolecular hydrogen bonds based on CPMD method. Further, classi-cal molecular dynamics was applied to investigate proteins. Here, we would like to report our results for two biomolecules. The first one is proteinase K for which the impact of mercury(II) on its catalytic center was studied. The second one is strep-tavidin. For the latter one its complexes with biotinylated ligands were investigated. We close our review with a paragraph describing further development and perspec-tives related to CPMD method.

Słowa kluczowe

cPMD, classical MD, intramolecular hydrogen bond, intermolecular HB, schiff base, mannich base, n -oxides, proteins

cPMD, klasyczna dynamika molekularna, wewnątrzczasteczkowe wiązanie wodorowe,, międzycząsteczkowe wiązanie wodorowe,, zasada Schiffa, zasada Mannicha, n -tlenki, białka