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QUANTUM-MECHANICAL BASED SIMULATIONS OF AN AMMONIUM ION IN AQUEOUS SOLUTION

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(Time New Roman 14) → *Ms. Patoomwadee Intaratep[1*], Assoc. Prof. Dr. Anan Tongraar[1], and Prof. Dr. Kritsana Sagarik[1]*

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Abstract : A molecular dynamics simulation based on combined ab initio QM/MM approach has been performed to investigate the properties of $NH_4^+ - H_2O$ complex in aqueous solution. By the QM/MM technique, the NH_4^+ ion and its first hydration sphere were treated at the Hartree-Fock level using DZV basis sets, while the rest of the system was described by classical pair potentials. It was found that the structure of the $NH_4^+ - H_2O$ complex was rather flexible and more disordered. The influence of the ion on the vibrational motions of its surrounding water molecules were evaluated by means of Fourier transformation of the velocity autocorrelation functions (VACFs) and the results were compared to those obtained by a QM/MM simulation of pure water.

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(Angsana 14) → การประชุมวิชาการบัณฑิตศึกษา มทส.. ครั้งที่ 2

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