



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Water contamination is a global issue in most parts of the world. The present thesis deals with the microscopic nature of interaction of two major water contaminants, namely selenium (Se) and arsenic (As), restricting largely to their relevant inorganic forms, owing to their higher solubility in water, employing ab initio molecular dynamics simulation. Various microscopic properties including molecular structure, hydrogen bonding, vibrational spectra, etc. are examined in detail. The thesis is organized as follows. A review of the state-of-the-art research activities on solvation studies of ab initio molecular dynamics, bio-geochemistry of selenium and arsenic species as well as the motivation for the present work is outlined in Chapter 1. Chapter 2 of the thesis summarizes the theoretical techniques employed in the work. Chapters 3 and 4 of the thesis present ab initio molecular dynamics studies on various inorganic Se – VI and Se – IV species in water. In chapters 5 and 6 inorganic As – III and As – V species are examined. Chapter 7 gives the conclusion of the thesis.