Topics in Computational Materials Science

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Topics in Computational Materials Science

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FOREWORD

The demands of understanding new experimental results for various types of growth, characterization of fascinating electronic devices and of striving effective guidelines for novel samples challenge computational materials science to make significant contributions. Among all the contributions in the past several years, I subjectively chose the following areas which are of current interests and are important for further advances:

- (1) Development of efficient computational schemes for first-principles and realistic simulations of surfaces.
- (2) The searching for ways to abate computational intensiveness in accurately determining the energy gap for semiconducting samples.
- (3) Investigation of microscopic properties of photonic devices.
- (4) Parametrization of interactions for large scale electronic calculations involving transition metal elements.
- (5) Modeling, by many-body Hamiltonians or phenomenological potentials, for Monte Carlo or molecular dynamic simulations.

This book concerns specific topics in the above five areas. These topics are both crucial to the development of future computational materials science and for providing better microscopic understanding of materials used to making innovative electronic devices. I am fortunate to have had the privilege of inviting prominent authors who are authorities in their respective areas to contribute chapters for reviewing the current status and delineating directions for future research.

The N-scaling scheme and parallel computing techniques are the principal elements for improving computational efficiency in realistic modeling involving a large number of atoms based on first-principles. They will be discussed in Chapter One by Dr. E. B. Stechel and in Chapter Two by Drs. J. S. Nelson and S. J. Plimpton. Professor S. G. Louie presents in Chapter Three the GW method for improving the semiconductor energy gaps over the results obtained by using the local density approximation of density functional theory; this improvement will provide meaningful comparisons with experimental data in the characterization processes. Since photonic devices are potential candidates for future device applications, photonic band calculations will be explained in Chapter Four by Drs. R. Biswas, M. M. Sigalas, C. M. Soukoulis,

and Professor K. M. Ho. We realize that there are vast amount of experimental results to be understood on transition metal surfaces and defects involving transition metal elements. In Chapter Five, the tight-binding method for calculating electronic properties of large systems involving transition metal elements will be described by Drs. M. Mehl and D. Papaconstantopoulos. The modeling approaches are state-of-the-art alternatives to the first-principles simulated annealing method of Car and Parrinello for treating alloy problems and surface morphologies. The crucial ingredient for the success of these approaches is the determination of realistic interaction parameters. For alloy problems, Dr. Z. W. Lu and Professor B. M. Klein contribute Chapter Six to demonstrate how to study alloy properties by the Ising model using inputs determined from first-principles calculations. Professor E. Kaxiras enunciates, in Chapter Seven, computational methods for investigating epitaxial growth of semiconducting surfaces. Dr. M. Fallis and I contribute Chapter Eight on modeling close-packed metallic surfaces using the so-called bond saturation model. The parameters characterizing the model are determined from the embedded atom method and are used in Monte Carlo simulations of morphologies of adatoms in homoepitaxial growth. As several authors emphasize, it is hoped that this book will not only benefit researchers in these areas but will also serve as a starting point for scientists to devise new and more powerful methods.

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C. Y. Fong

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