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Computational Methods in Material Science

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The current revolution in Materials Science leading to vast advances in pre-existing and emerging technologies had significantly impacted all aspects of our modern life. The continuous efforts in searching for new functional and smart materials facilitated the design of miniaturized and more efficient devices, and led to great advancements in pharmaceutical, medicinal, agricultural, energy related industries, and many more. Before employment in a given application, a newly developed material needs to be fully characterized and tested for efficient delivery and fulfillment of industrial and technological requirements. This calls for establishing experimental setups equipped with modern testing facilities that could be exceedingly expensive, and time consuming. In addition, the cost of materials for experimental work could be high in some cases. The financial limitations, however, make it difficult to construct such facilities for a large fraction of researchers worldwide, especially in nations with limited financial resources. Accordingly, computational techniques have been developed to provide efficient materials characterization, and design of smart materials and devices for practical applications at a relatively low cost. These techniques are also crucial in providing detailed information about the structural and physical properties of the material at the molecular level, thus allowing for better understanding of how the material functions, and facilitating the tuning and improvement of the material's characteristics for a specific application. However, comparison of the results of the computational techniques with experimental results is crucial to examine the reliability of the computational techniques, at least in its initial stages.

This special issue is dedicated to a collection of articles concerned with the employment of computational techniques in materials science. In these contributions, first-principles density functional theory was adopted to investigate the structural, electronic, and spectroscopic properties of materials for photovoltaic,

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and pharmaceutical and medicinal applications. Some of the featured articles also included experimental results, and main conclusions were drawn based on the theoretical and experimental parts of the study. This collection of articles may open doors for future computational work on relevant advanced materials.