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The Fate of Molecular Systems at High-Pressure

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Message from the Guest Editors

Dear Colleagues,

Pressure is an incredibly powerful tool for tuning interactions among molecules to make them comparable to intramolecular interactions. Besides the intermolecular distances, relative molecular orientations and conformations can also be changed with major consequences for the electronic density redistribution. Many different phenomena ranging from structural phase transitions to chemical reactions, including metallization and the emergence of exotic magnetic or superconductive phases, are observed as a consequence of the internal energy increase.

The aim of this Special Issue is to present a collection of articles depicting some of the most recent findings achieved by compressing molecular systems in DACs and in computer simulations. Ideally, this collection should give an overview of the rich variety of transformations occurring under high-pressure conditions, encompassing many different research areas and topics in both fundamental and applied sciences.

Prof. Dr. Roberto Bini
Prof. Dr. Mario Santoro
Guest Editors



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Special Issue



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Message from the Editor-in-Chief

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