



## Metallic Systems: A Quantum Chemist's Perspective

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**Metallic Systems: A Quantum Chemist's Perspective** From Brand: CRC Press

Metallic systems are ubiquitous in daily life. They play key roles, for example, in the chemistry of many biomolecules, ionic solutions, nanoparticles, and catalytic processes. They may be in solid, liquid, or gaseous form. The interactions of other molecules with metal surfaces are of considerable importance. Each of these topics is addressed in **Metallic Systems**. As we have entered the age where theoretical approaches are sufficiently mature to complement and guide experiments in many areas, an understanding of the theoretical tools and approaches to studying metallic systems is essential. **Metallic Systems** is concerned with enhancing our understanding of the diverse chemistry of metals and metal-containing systems and the applicability of modern quantum chemistry methodologies to study them.

**Metallic Systems** presents brief overviews of most of the popular approaches to quantum chemical treatments and computations of chemical systems that include metals. Attention is given to the potentialities and limitations of first principles Density Functional Theory and dynamics methods (e.g. QM/MM approaches). The book emphasizes the importance of using methods that take into account crucial physical features such as explicit solvation, temperature and dynamics of metal-containing systems. It emphasizes first principles calculations in providing reliable and detailed information concerning electronic structures, mechanisms, and reaction energetics.

Accessible to newcomers to the field, **Metallic Systems** overviews theory underpinning current methodologies. It presents a practical set of modalities for studying metallic systems, assesses current technological barriers, and examines future challenges and topics of exploration.



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