

Bonding, Structure, and Performance of Two-Dimensional Materials

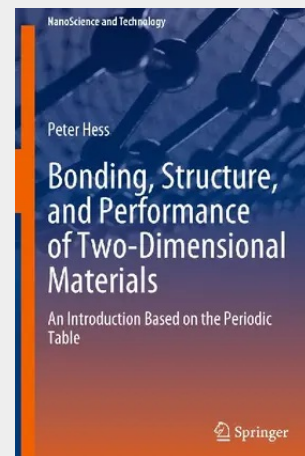
An Introduction Based on the Periodic Table

This book presents a wealth of results obtained by first-principles calculations, molecular dynamics simulations, and tight-binding modeling on two-dimensional covalent bonding and the resulting formation of 2D materials. It focuses on the bonding–structure relationships derived from the periodicity of the electron configuration and atomic size, paying particular attention to the overall stability of various elemental and composite networks. In addition to accurate first-principles calculations, the book uses a linear combination of atomic orbitals and the hybridization concept to gain deep insight into the rules governing the world of 2D chemistry.

Of special interest are the novel properties of 2D materials based on quantum confinement effects in two dimensions and the large surface-to-volume ratio. The book gives an introduction to the fundamental principles of 2D structure formation for newcomers in this field, simultaneously providing a comprehensive source of data on bonding strength, geometrical structure, and nanomechanics characterizing the manifold of chemical networks in two-dimensional space. This book is a valuable reference for material scientists, chemists, and any researcher in the field of 2D materials and low-dimensional nanoscience.

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