

# The Chemical Bond: Fundamental Aspects of Chemical Bonding

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This is the perfect complement to "Chemical Bonding - Across the Periodic Table" by the same editors, who are two of the top scientists working on this topic, each with extensive experience and important connections within the community.

The resulting book is a unique overview of the different approaches used for describing a chemical bond, including molecular-orbital based, valence-bond based, ELF, AIM and density-functional based methods. It takes into account the many developments that have taken place in the field over the past few decades due to the rapid advances in quantum chemical models and faster computers.

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#### **Editorial Review**

#### Review

"The two volumes would serve upper-level undergraduates who are well versed in mathematics and chemistry, but they are most suitable for graduate students, faculty, and researchers in chemistry. The exhaustive chapter references make each book a useful go-to reference source. Highly recommended. Upper-division undergraduates, graduate students, and researchers/faculty." (*Choice*, 1 May 2015)

#### From the Back Cover

One of the fundamental territories of chemistry is the chemical bond, the glue from which an entire chemical universe is constructed. For a while it seemed that Chemists have, by and large, abandoned their territory as if everything about bonding is known and well understood; the frontier has moved to Nano and Bio, leaving the original territory untended. This however was a wrong impression, since the interest in bonding has quickly revived to be accompanied by many interesting theoretical approaches to probe the origins of bonds, many novel bonding motifs, and even experimental studies that describe imaging of bonds being broken and remade using atomic force microscopy. The bond is becoming again a central intellectual arena. Enormous progress was made in recent time in method development which gives insight into the chemical bond using calculated numbers which come from sophisticated quantum chemical methods in line with the famous statement of Charles Coulson: "Give us insight not numbers". This "return of the bond" has prompted the two editors to edit these two volumes on bonding, and it is only fitting that their publication date is close to the centenary of the Lewis seminal paper on electron pair bonding. The two volumes are meant to attract the interest of the practicing chemist, teachers and advanced students who may want to learn about the present understanding of chemical bonding.

Volume 1 contains eleven chapters, which provide the theoretical frameworks of the various perspectives on bonding, coming from VB and MO theories, ELF, AIM, NBO, BLW and EDA. This Volume lays the foundations for the applications across the periodic table.

#### About the Author

Gernot Frenking studied chemistry at the Technical University Aachen (Germany). He then became a research atudent in the group of Prof. Kenichi Fukui in Kyoto (Japan) and completed his PhD and his habilitation at Technical University Berlin (Germany). He was then a visiting scientist at the University of California, Berkeley (USA) and a staff scientist at SRI International in Menlo Park, California (USA). Since 1990 he is Professor for Computational Chemistry at the Philipps-Universit?t Marburg.

Sason Shaik is a graduate of the University of Washington (USA), where he also obtained his PhD. After a postdoctoral year at Cornell University, he became Lecturer at Ben-Gurion University of the Negev (Israel), where he became Professor in 1988. In 1992 he moved to The Hebrew University where he is Professor and the Director of the Lise Meitner-Minerva Center for Computational Quantum Chemistry.

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