

# ACCMS-Global Research Center

## SRMIST, Chennai India


### Webinar #9



### Prof. Richard Dronskowski

Chair of Solid-State and Quantum Chemistry, RWTH Aachen University, Aachen, Germany

**Title: Extracting Bonds from Bands: COHP and other Chemical-Bonding Tools via LOBSTER**

 31<sup>st</sup> May 2022, 12.30 – 2.00 pm IST

Registration link: <https://tinyurl.com/mr4yk8tn>

### Biography

Prof. Dr. Richard Dronskowski graduated in 1990 from University of Stuttgart and got his Habilitation in 1995 from University of Dortmund. He worked with Nobel Laureate Prof. Roald Hoffmann. In the late nineties he joined RWTH Aachen where he served as the Director of the "Anorganische Chemie" and the Chair of the Solid-State and Quantum Chemistry Group. During the past two decades or so, he has succeeded in establishing a vibrant multidisciplinary group of chemists, physicists, computer scientists in Aachen. He also served as Senior Scientist in MPI Stuttgart, guest professor in Tohoku University, and more recently as "Distinguished Chair Professor" of the Hoffmann Institute of Advanced Materials, in Shenzhen (China) since 2018. He received various awards which include the Otto Hahn Medal of the Max Planck Society, Innovation Award of RWTH Aachen, etc., and is decorated with various professional memberships such as, German Chemical Society, American Chemical Society, German Physical Society and the German Crystallographic Society. He is Editorial Board members of several journals including J. Solid State Chem., Inorganics, J. Phys.: Condens. Matter, and is also a member of the Scientific Advisory Board of the European Spallation Source. His research interests span a wide cross section ranging from Quantum Chemistry to Synthetic Solid State Chemistry to Chemical Crystallography. His research group has made significant contributions to both methodology development as well as applications, e.g. in understanding of chemical bonding, phase predictions, thermochemistry, neutron diffraction etc. He has more than 530 publications with h-index of 60. He is the originator of the COHP method for quantitative analysis of chemical bonds, and also leads the team for the LOBSTER software package. In 2005 he authored the well known treatise on "Computational Chemistry of Solid State Materials" published by Wiley-VCH.

### Abstract

What makes atoms stick together in molecules and solids, exactly? To answer that, population analysis as imagined by Mulliken (1955) has held a prominent place in quantum chemistry for decades already. Likewise, periodic bonding indicators such Crystal Orbital Hamilton Population, COHP (1993) have been helpful, the latter carried out using local-basis codes. Such analysis has allowed to *chemically* understand three-dimensional Peierls distortions, spin polarization in itinerant magnets, and a lot more. While plane-wave packages such as VASP, ABINIT, Quantum ESPRESSO etc. offer computational advantages, they lack locality, so the aforementioned chemical concepts were unavailable. Nonetheless, all local bonding information can be analytically reconstructed by transferring plane-wave pseudopotential data to local auxiliary bases built from contracted Slater-type orbitals, as implemented in the LOBSTER (Local-Orbital Basis Suite Towards Electronic-Structure Reconstruction) code, freely available at [www.cohp.de](http://www.cohp.de), and it also offers other tools like the density-of-energy, crystal-orbital bond index, as well as established quantum-chemical descriptors such as Mulliken or Löwdin charges directly from the wavefunction, not indirectly from the density. All that will be illustrated, using essentially non-mathematical reasoning, from a variety of recent examples, including elemental solids, simple molecules, battery and "metavalently" bonded phase-change materials.

### Panelists



**Prof. Kaoru Ohno**  
Yokohama National University  
Japan



**Prof. Umesh Waghmare**  
JNCASR, Bangalore  
India



**Prof. Jer-Lai Kuo**  
IAMS, Academia Sinica  
Taiwan

Zoom meeting details will be shared with the registered participants

#### Convener:

**Prof. Yoshiyuki Kawazoe**  
Head, ACCMS-GRC  
SRMIST, KTR

#### Organizers:

**Dr. V.J.Surya and Dr.S. Yuvaraj**  
ACCMS-GRC Center-in-Charges  
Department of Physics and Nanotechnology,  
SRMIST, KTR