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## Webinar-36

Asian Consortium on Computational Materials Science (ACCMS) Centre  
SRM University-AP, Amaravati, Andhra Pradesh, India

**September 30, 2025 | 11:30 AM - 01:30 PM (IST)**

Webinar Zoom link:

<https://srmap.zoom.us/j/91831904565?pwd=tga2BbaeVogTkudlip6FxJdBFdc3tA.1>  
Meeting ID: 918 3190 4565, Passcode: 393399

**Title:** Localised Molecular orbitals in Mott insulators  $\text{GaTa}_4\text{Se}_8$  and  $\text{Nb}_3\text{Cl}_8$

### Abstract:

Atomic orbitals and molecular orbitals in solids are no longer well defined due to periodical translation symmetry, but they are still the best basis sets for understanding and constructing low-energy effective models. They are natural and present physically intuitive images. In some solids, molecules or clusters form the most basic structural units, in which the electron distribution follows molecular orbitals rather than atomic orbitals, with deviations from atomic positions, higher orbital angular momentum (different from the angular momentum of the orbitals), Similar local characteristics and other characteristics. In this talk, I will introduce how to use group representation theory and Wannier function theory to construct molecular orbitals in solids, and how to use molecular orbitals to study two molecular orbital Mott insulators, namely  $\text{GaTa}_4\text{Se}_8$  and  $\text{Nb}_3\text{Cl}_8$ , to demonstrate ideal multi-band and the implementation of the single-band Hubbard model in materials composed of these transition metal electronics.

### References:

- [1] H. Weng et al., Phys. Rev. B 92, 045108 (2015).  
[2] S. Zhang et al., Phys. Rev. B 102, 214114 (2020).

- [3] S. Gao et al., Phys. Rev. X 13, 041049 (2023).  
[4] X. Huang et al., Newton (2025).

### Short Biography:

Hongming Weng, Professor of Physics at the Institute of Physics, Chinese Academy of Sciences (CAS), and director of the Condensed Matter Physics Data Center, CAS. He received his undergraduate degree from the Department of Physics of Nanjing University in 2000 and his PhD in condensed matter physics from Nanjing University in 2005. He works in the direction of computational condensed matter physics. In addition to the development of computational methods and programs, he focuses on the computational research of novel quantum phenomena of solids, including topological materials, diluted magnetic semiconductor and transition-metal compounds. His papers on theoretical prediction and experimental discovery of Weyl semimetals were selected into the collection to celebrate 125th anniversary of Physical Review journals by American Physical Society. He received Nishina Asia Award 2017, Xplorer Prize 2022 and the First Prize of National Natural Science Award.



**Prof. Hongming Weng**

*Director of the Condensed  
Matter Physics Data Center,  
Chinese Academy of Sciences*



**Panelist :-**

**Prof. Ranjit Kumar Nanda**

*Professor, IIT, Madras.  
Department of Physics*

### Conveners:

Prof. Yoshiyuki Kawazoe, Head, ACCMS-Centre  
Prof. G. P. Das, TCG Crest  
Prof. Ranjit Thapa, SRM University -AP

### Local Organisers:

Dr Mahesh Kumar Ravva, SRM University-AP  
Prof. Umesh Waghmare, JNCASR  
Dr Surya VJ, ACCMS