

When: May 31, 13:00-14:00 Where: Skoltech, blue building, room 403

Sn<sub>2</sub>Br<sub>2</sub>SiS

Computational Materials Science Seminar

Inorganic

double helix

# **First Principles Studies of Novel Inorganic Double Helices and Thin Layers of Perovskites**

## Abstract

I will present our recent results on some novel one- and two-dimensional structures using first principles calculations.

### This will include:

**1)** One dimensional inorganic double helices of the type  $A_2B_2XY$  (A = Si-Pb, B = Cl-I, and XY = PN and SiS). A representative structure is shown in the figure. In these structures a helix of the halide of a group-IV element wraps around the PN or SiS helix and the two are interconnected [1]. All these double helices are semiconducting and in many cases the band gap is direct which makes them interesting for optoelectronic applications.

2) Thin layers (one to six unit cell thick) of inorganic halide perovskites with stoichiometry  $A_{n+1}M_nX_{3n+1}$  (n = 1 – 6, A= Cs, M = Pb and Sn, and X = Cl, Br, and I) which are attracting great interest. All these layers have a direct band gap [2] and this is promising for solar energy as well as optoelectronic applications. Our studies show that layers with n > 3 can give stability comparable to bulk counterparts and that the thickness as well as the choice of the elements allows one to tailor the properties of these systems. If time will permit, I will present some recent results on boron nanostructures [3-5].

Acknowledgements: I gratefully acknowledge my collaborators T.K. Bijoy, A. Bala, A.K. Deb, A.B. Rahane, P. Saha, N. Sukumar, J. Karthikeyan, Y.S. Ranawat, and P. Murugan, who contributed to these studies. The calculations were performed using Magus at SNU and CECRI machines as well as resources at VKF. Financial support from ITC-PAC and DST is thankfully acknowledged.



**Speaker:** Dr. Vijay Kumar Foundation, 1969 Sector 4,

Gurgaon, Haryana 122001, India.

Center for Informatics, School of Natural Sciences, Shiv Nadar University, Tehsil Dadri, Gautam Buddha Nagar, Uttar Pradesh 201314, India.



#### References

[1] T.K. Bijoy, P. Murugan, and V. Kumar, Phys. Chem. Chem. Phys. 20, 10060 (2018). [2] A. Bala, A.K. Deb, and V. Kumar, J. Phys. Chem. C122, 7464 (2018). [3.] A. B. Rahane and V. Kumar, Nanoscale, 7, 4055 (2015) and to be published. [4] P. Saha, A.B. Rahane, V. Kumar, and N. Sukumar, J. Phys. Chem. C121, 10728 (2017). [5] J. Karthikeyan, Y.S. Ranawat, P. Murugan, and V. Kumar, to be published.

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## Biography

Prof. Vijay Kumar did Ph.D. from University of Roorkee in India and was a Humboldt Fellow at Free University, Berlin. He joined IGCAR Kalpakkam in 1985 and was invited as a Staff Member of ICTP Trieste where he coordinated the Diploma Course in Condensed Matter Physics (1991-93). He was visiting Professor in CNRS, Orsay, visiting scientist in Cavendish Laboratory, SISSA, and AIST, Tsukuba, and Guest Professor in Tohoku University. He is at the Dr. Vijay Kumar Foundation in Gurgaon and Research Professor in Shiv Nadar University. He has published ~ 200 papers and edited four books. He received Materials Research Society of India (MRSI) Medal (1996) and ACCMS Award (2004). He initiated the subject group "Computer Aided Design of Materials" in MRSI and was its first Chairman. Currently he is working on nanomaterials, energy materials and hard materials.