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#### CV

Chemistry major and PhD at Chemistry Faculty of the Lviv State University, Ukraine.

Faculty staff with academic appointment of assistant professor, associate professor, vice-president at the Lviv State University.

Researcher at the Max-Planck-Institut für Metallforschung and the Max-Planck-Institut für Festkörperforschung in Stuttgart, head of research group at the Max-Planck-Institut für Chemische Physik fester Stoffe in Dresden, Germany.

Since 2001- Scientific Member of the Max Planck Society and Director at Max-Planck-Institut für Chemische Physik fester Stoffe (Department Chemical Metals Science) in Dresden, faculty member and honorary professor in chemical metal science at the Dresden University of Technology, Germany.

Guest professor at the University of Rennes, at and ENSICAEN, Caen, France, as well as the Chinese Academy of Sciences and University of Shanghai, China.

Doctor philosophiae honoris causa of the National Academy of Sciences of Ukraine.

V. I. Vernadsky Gold Medal of the National Academy of Sciences for the outstanding achievements in thermoelectric materials science

**Giovedì 13 ottobre 2022**

**Aula 2**

**ore 14.30**

#### ***Chemical bonding and properties of intermetallic compounds***

#### **Abstract**

Intermetallic compounds reveal chemical and physical behaviors interesting for applications and may serve as basic components for materials design. In particular chemical catalysis, thermoelectric or heavy-fermion behaviors are in focus recently. An attempt to find a direct link between the properties and the crystal structure as well the atomic interactions for this group of inorganic substances reveals often a lack of reliable information on all three. For interpretation of their chemical and physical properties a better understanding of the composition and bonding in crystal structures of these substances is necessary. Especially the understanding of chemical bonding is recently in focus of research. An application of new quantum-chemical tools opens the way to systematic real-space definition of the basic categories for chemical bonding description like atomic charges, covalence, ionicity, polarity of bonding etc.

Spatial distribution of regions with different types of chemical bonding – bonding inhomogeneity and anisotropy - influences especially the thermal transport in intermetallic compounds. It also helps in understanding of the electronic counts necessary to stabilize the (pseudo) band gap and the strong DOS gradient at the Fermi level the analysis of chemical bonding using the electron-localizability approach, make the quantitative description of the surface state and estimation of the adsorption energies of certain adsorbates possible, allowing the interpretation of the experimentally obtained catalytic results.

To find out how to reach the Department, go to <http://www.chimica.unige.it>. For further informations on this specific seminar or in order to ask for an appointment with the speaker after or before the seminar, contact Prof.ssa Serena De Negri ☎ +39 0103536159 e-mail: [serena.denegri@unige.it](mailto:serena.denegri@unige.it)