THEORETICAL INSIGHT INTO THE SINGLE-LAYER SYSTEMS EXHIBITING STRONG ANTIFERROMAGNETIC COUPLING - A QUEST FOR PRECURSORS OF NOVEL SUPERCONDUCTORS

ABSTRACT FOR THE GENERAL PUBLIC

MOTIVATION. Quest for advanced materials is an abiding interest of rapidly developing modern society, seeking a convenient solution of numerous technological obstacles. Many of today's problems could be solved by reducing electricity transmission loses, making transport faster and cheaper, enabling efficient energy and information storage and reducing costs of instrumental analyses in medicine. The material addressing these challenges is called a **superconductor**, that is a substance which may transfer electricity without any energy loss. Although such materials are already known, and even applied in certain fields of science and technology, yet they require cooling to very low temperature to function properly. The best of those works only at temperatures lower than –135 °C, the temperature not found even on the chilliest place on Earth. Amazingly, at ambient pressure conditions (*i.e.* 1 atm at the surface of our planet) only **one family** of superconductors is capable of transmitting electric current without any loss while cooled with a cost-efficient cooling medium, liquid nitrogen (above –196 °C). These are so-called **high-temperature** superconductors, which always contain copper and oxygen (among other chemical elements) in their composition. They were discovered nearly 35 years ago resulting in the Nobel Prize for this discovery. Unfortunately, to date no other family of similar bulk compounds was found. While there is no final consensus in the community what makes these materials so unique, they are good indications that an interplay between **magnetic** and electron-electron interactions (with a nontrivial component originating from atomic lattice **motions**) jointly "glue" the current-conducting electrons and contribute to the success of these unparalleled systems. Repeating and surpassing their success would constitute an undisputed breakthrough in the field, and help us to learn in-depth the mechanisms of superconductivity in general.

INSPIRATION. Recent theoretical and experimental analyses have pointed out a new family of precursors that mimics the behaviour of before-mentioned copper-based compounds. These novel systems contain **silver** instead of copper, and **fluorine** instead of oxygen. The latest computational findings indicate that formation of a flat layer containing silver and fluorine atoms may greatly enhance their properties. The trick consists of depositing them in the form of a **single atomic layer** on appropriate crystal surface. The thorough estimate is that such systems might superconduct at temperatures close to –80 °C, which would set a **historical record**. Experimental verification of these predictions is ongoing.

The deliberate design (*i.e.* manipulating features of materials at atomic level) is actually long known, and it has proved to be successful in reaching the desired properties. This approach is described by a buzzword "nanotechnology". **Theoretical calculations** play a key role in nanotechnology since they enable low-cost predictions of materials properties. This allows one to select the most promising systems before major funds and human resources are involved in experimental studies.

GOALS AND METHODS. The main **goal** of this research project is to find yet **other layered precursors** of as yet unknown families of superconducting materials. Concept of the work is based on computational modelling of systems which contain an odd number of electrons on metal centre (Ni^{1+}, Yb^{3+}, Ti^{3+}) and are known to exhibit **"strong" magnetic properties** when combined with certain non-metal elements. Moreover, their "non-magnetic" analogues (Pd^{2+}) and those in between which may "be magnetic" or not (Ni^{2+}) will also be studied as valuable reference systems. We will place **layers "A"** containing these cations and anions (O^{2-}, S^{2-}, Cl^{-}, H^{-}) on the surface of many different **substrate** materials and use supercomputers to calculate the preferred position of atoms, and the resulting physical properties. The properties will crucially depend on the substrate material, which will allow us to select **optimum systems** similar to the above-mentioned copper- or silver-based materials. In the second step we will model modified systems containing yet another atomic **layer "B" nearby** which is capable of either injecting or withdrawing electrons from the layer "A" of interest (this process is called **doping**). Finally, for all these systems at different doping levels, and in the collaboration with worldwide-recognized foreign experts from Italy and China, we will calculate the temperatures at which these materials could superconduct. Eventually, the most promising complex system will be selected.

EFFECTS. Positive **outcome** of the project, *i.e.* surpassing the value of –80 °C predicted before for atomic layer of silver fluoride, and possibly approaching the **room temperature**, may hopefully pave the way towards experimental tests in various laboratories. If these properties will be confirmed in the future, it might change the ways our society as a whole, and every human, deals with all electric current appliances. Widespread use of superconductors in CPU fabrication would lead to construction of even faster computers. Whereas associated energy savings would improve the **environment** of our planet thanks to reduction of fossil fuel combustion worldwide.