Background. In our daily life we utilize a large numer of electronic devices, some of which we even fail to recognize. All of them are macroscopic. Inside them are complex microscopic devices invented by humans, such as a galvanic cell (inside a lithium battery), a capacitor (in a backup power supply or ignition system of a car), an n-p junction (in a solar cell), or a field-effect transistor (in central processing unit of our computers). In 2021, an entirely new type of device was proposed by one Italian and two Polish scientists. The device is smaller than its predecessors (that is, a nano-device) and has different functionalities from those mentioned above. It is called chemical capacitor, or shortly chem-cap. Chem-cap is composed of four chemical substances: one is called a substrate, and the remaining ones may be grown on it, the next one is called a charge reservoir, and it is electron-rich, the following one is a separator, and the last one is electron-hungry. Eventually, a protective fifth one may be added on the top. One key feature is that if a separator was not introduced, an extremely vigorous (even explosive!) reaction would take place between electron-rich and electron-hungry materials. While this novel setup has so far been theorized, there is a preliminary example from the literature that such device could indeed be fabricated using modern technological approaches.
Reasons for attempting a particular research topic. As with every new scientific toy, there come surprises, successes, failures and risks. And one should understand it well before it enters some of our daily life macroscopic devices. Preliminary work has revealed that chem-cap features a combination of many unique features, which are not exhibited by related devices. The key one is possibility to smoothly inject large amount of electrons to or from virtually any type of material. Even if starting materials did not conduct electric current well, they will become good conductors (metals) upon injection; the whole functionality is dependent mainly on chemical composition of electron-hungry and electron-rich layers, and the thickness and other properties of the separator. Therefore, to understand the limits of properties achievable in such a device, one should study many different compositions and types and thicknesses of a separator. This is most easily and inexpensively done these days using supercomputers which permit very advanced calculations to be performed. The outcome of these calculations (based on so called quantum theory) is usualy very close to what would be observed in experimental reality. Such theoretical study is proposed in the current project. The **project goal** is to screen a large numer of chemical compositions and understand most fundamental features and functionalities of chem-cap devices built from them. This will save great deal of time and at the end of the project we will be able to say which metarials combinations might exhibit desired features and thus be useful for technological purposes. The compositions are limited only by fantasy!
Description of research. The key functionalities studied studied will be superconductivity (i.e. conducting current without any resistance), magnetoresistance (i.e. large changes of electric conductivity if magnetic field is varied), solar energy harvesting and performing chemical reactions on a metallic surface with great ease (called catalysis). We are in principle unrestricted in terms of chemical materials applied, and may vary chemical composition of chem-cap constituent in a very broad range. **Substantial results expected.** The most ambitious scope of the project is to theoretically predict superconductivity in thin-layer materials containing hydrogen, named hydrides, at temperatures *exceeding room temperature, and in the absence of any external pressure*. Preliminary evaluations suggests that temperature values up to 830 ^{o}C (or ca. 1100 K) are possible, and even a third of this value would mean a technological breathrough. If engineered in the future, such discovery would bring immense consequences for contemporary science, technology and civilization (facile magnetic levitation transport, transfer of huge amounts of electric current without losses and heat dissipation to the environment, ultra-fast computing, etc.). The chem-cap devices could be fabricated similarly to those based on n-p junctions which we already prepare on the industrial scale. Another important result foreseen is that we will be able to turn some inexpensive abundant metals such as e.g. copper into good catalysts (for example in reactions were hydrogen is added or removed from a molecule), which was quite impossible before.
The project is divided in 4 workpackages, and covered by 8 distinct Tasks. Personell consists of the Principal Investigator (Grochala), one postdoc, two PhD students, two international collaborators, Lorenzana (Italy) and Zurek (USA), and Hoffmann (USA) as advisor. Grochala and Lorenzana are senior inventors of chem-cap device and they would like to substantially expand that idea.
Deliverables. The material outcome of the project will consist of at least 5 prescriptions (i.e. given chemical compositions) which merit experimental studies, in particular three of those which may deliver room-temperature superconductivity, one for efficient light harvesting, and one for catalytic reactions. The results will be published in scientific papers, and public outreach will be ensured.