学术报告

题　目： **1. Strongly Confined, Simple Molecular Systems at High Pressures**

2. Carbon Dioxide at Extreme Eonditions

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地　点： **中科院固体物理研究所 新楼 520 会议室**

Abstract:

M. Santoro: In this seminar I will talk about a recent part of my research, yet a very intriguing one, which joins my well established experience on high pressure science of simple molecular systems to the amazing world of zeolites. I will first present on several novel compounds obtained by reacting simple carbon bearing molecules at high pressures (HP) in the sub-nanopores of two non-catalytic, pure SiO2 zeolites: silicalite-1 and ZSM-22. I will show a CO2-SiO2 compound, a disordered silicon carbonate1, obtained by reacting silicalite and nano-confined CO2 at about 20 GPa and 600-1000 K. The discovery of silicon carbonate reveals unique oxide chemistry at high pressures and the potential for synthesis of a class of previously uncharacterized materials. I will then report on HP (GPa) polymerization of ethylene, acetylene and CO in the zeolites, leading to novel nanocomposites, all recovered at ambient conditions. Indeed, a polyethyelene/silicalite composite was formed with tunable thermo-mechanical properties and potential null thermal expansion2. Then, we obtained a polyacetylene(PA)/silicalite composite, where branched, semiconducting oligomers are confined in the protecting zeolite3. We also obtained 1D PA in the 1D host channels of ZSM-224. In this composite, PA is expected to exhibit a peculiar quantum behavior related to the 1D confinement, which could lead to technological applications. I will then show polymerization of CO in both zeolites4,5, leading to more chemically and structurally ordered polymers than obtained in polymerization of bulk CO. PolyCO/zeolites could constitute a new class of energetic materials. Finally, I will show recent unpublished results on HP confinement of dense O2 and N2 in zeolites, aimed to investigate nano-phases of these systems. Remarkably, confined O2 and N2 show similar intermolecular interactions than in bulk sample at the same pressures, which seems to be an universal property of confined simple molecular systems in purely siliceous zeolites. In particular, confined O2 shows molecular clustering as in bulk O2 samples, whereas polymeric, confined forms of nitrogen are in view as in bulk nitrogen. Investigations involved high temperature diamond anvil cells, optical spectroscopy, and X-ray diffraction.

Federico Aiace Gorelli: The investigation of the phase diagram of carbon dioxide at extreme pressures and temperatures has resulted in the last decades in the experimental discovery of several crystalline polymorphs, and even amorphous forms (a-carbonia), ranging from molecular solids to fully extended covalent solids with crystal structures similar to those of silicate minerals of pure silica (phase V). The discussions on their thermodynamic stability, on the transformation of the chemical bonding leading to 4-fold and even 6-fold carbon coordination at extreme pressures and on the P-T path followed to obtain these phases has stimulated many simulation works and a rich literature. The prediction of exotic layered structures at high pressures, the possibility to recover the non molecular 4-fold coordinated phase V at ambient pressure and the existence of other amorphous forms apart from a-carbonia are only some examples of hot topics of condensed matter physics. I will show the most relevant aspects of this research for a general audience.

两位报告人是高压化学领域的专家，在 Nature, Nature Communications, Nature Physics, Physical Review Letters 等国际顶尖期刊发表文章数十篇。

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