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**High Pressure Phases of CaCO<sub>3</sub>, S and H obtained by USPEX.** Colin W. Glass\*, Artem R. Oganov, Lab. of Crystallography, ETH Zürich, Wolfgang-Pauli-Str. 10, 8093 Zurich, CH, coglass@student.ethz.ch.

Recently we have developed a very efficient and reliable method for crystal structure prediction [1,2], merging an evolutionary algorithm with *initio* total-energy calculations. Relying purely on theoretical knowledge and being thus independent from experiment, this method allows prediction of the most stable crystal structure at any given *P-T* conditions. Simultaneously it finds a large number of competitive metastable structures and gives an insight into the structural chemistry of the compound.

Focus here is on the results from USPEX on CaCO<sub>3</sub>, S and H at high pressure. For CaCO<sub>3</sub> we have discovered new stable structures between 42 and 137 GPa and above 137 GPa [3]. For S competitive metastable and a new stable structure around 5 GPa will be presented. In the case of H we show results from runs at 600 GPa, where contrary to conventional wisdom we have found only molecular structures.

[1] Glass C.W, Oganov A.R., Hansen N. (2006). USPEX: evolutionary crystal structure prediction

[2] Oganov A.R., Glass C.W. (2006). Crystal structure prediction using *ab initio* evolutionary techniques: principles and applications. Submitted.

[3] Oganov A.R., Glass C.W., Ono S. (2006). High-pressure phases of CaCO<sub>3</sub>: crystal structure prediction and experiment. *Earth Planet. Sci. Lett.* **241**, 95-103.