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Computational Design of Novel Compounds and Room-temperature Superconductors at High Pressure Conditions

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Pressure, which is a fundamental thermodynamic control on materials' properties, reduces inter-atomic distances and profoundly modifies electronic orbitals and bonding patterns. High pressure has been a versatile tool for creating exotic materials that are not accessible at ambient conditions. Recently, crystal structure prediction has played a leading role in major high-pressure discoveries. Among various structure prediction methods, CALYPSO method [1] (http://www.calypso.cn) is developed on top of swarm-intelligence algorithms by taking the advantage of swarm structures smart learning. Application of CALYPSO into prediction of high-pressure structures has generated a number of exciting discoveries. Examples point to the predicted chemical reactions of Fe/Ni-Xe and Au-Li at high pressures with the formation of unusual compounds Fe_3/Ni_3Xe and $AuLi_4/Li_5$, respectively [2-3]. Motivated by our theory, the Fe_3/Ni_3Xe compounds were recently experimentally synthesized, providing a possible solution on "missing Xe paradox" towards to Xe storage inside Earth core. Here, Au loses its chemical identity, and acts as a 6p element by achieving high negative oxidation state ($\geq$-2). Our prediction of high-T_c superconductivity on highly compressed H_2S [4] initiated the recent experimental observation of record high 200 K superconductivity in H_3S. Perspective towards to the design of room-T superconductors in compressed H-rich materials will be presented, including design of high T_c (>100 K) superconductor of TeH_4, the highest H-content superconductor in chalcogen hydrides [5]. References: [1] Y. Wang, J. Lv, L.Zhu, and Y. Ma, Phys. Rev. B 82, 094116 (2010); Comput. Phys. Commun. 183, 2063 (2012). [2] L. Zhu, et al, Nature Chem. 6, 644 (2014). [3]G. Yang, *et al.*, J. Am. Chem. Soc. 138, 4046 (2016). [4] Y. Li, et al, J. Chem. Phys. 140, 174712 (2014). [5] X. Zhong, *et al,* Phys. Rev. Lett. 116, 057002 (2016).