

Abstract Submitted  
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**Novel chemistry of matter under high pressure** MAOSHENG MIAO, Beijing Computational Science Research Center — The periodicity of the elements and the non-reactivity of the inner-shell electrons are two related principles of chemistry, rooted in the atomic shell structure. Within compounds, Group I elements, for example, invariably assume the +1 oxidation state, and their chemical properties differ completely from those of the p-block elements. These general rules govern our understanding of chemical structures and reactions. Using first principles calculations, we demonstrate that under high pressure, the above doctrines can be broken. We show that both the inner shell electrons [1] and the outer shell empty orbitals [2] of Cs and other elements can involve in chemical reactions. Furthermore, we show that the quantized orbitals of the enclosed interstitial space may play the same role as atomic orbitals, an unprecedented view that led us to a unified theory for the recently observed high-pressure electride phenomenon [3]. [1] M. S. Miao, *Nature Chemistry*, 5, 846 (2013). [2] J. Botana and M. S. Miao, *Nature Communications*, 5, 4861 (2014). [3] M. S. Miao and R. Hoffmann, *Accounts of Chemical Research*, 47, 1311 (2014).

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