Chemical Processes under Pressure

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Pressure dramatically affects the electronic structure of a material that modifies its structure and properties. Significant rearrangement of the electron topology due to the increase of electron repulsion in the compressed phase is expected and predicted by theoretical calculations. A simplistic model based on charge transfer between the elements has been used for binary compounds to rationalize the structure changes. We examine this proposal by analyzing the electron distributions extracted from experimental diffraction patterns and compare with detailed theoretical calculations of two binary alloys. The new information reveals the actual process is more complicated than anticipated. A consequence of electron rearrangement is the changes in chemical bonding and chemical reactivity. We examined the X-ray Raman spectra of silica, borate and carbonate glasses to search for signatures indicating substantial changes in the local bonding environment. Finally, potential chemical reactions between hydrogen with silica and carbonates at high pressure are investigated with theoretical calculations.