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High Pressure Chemistry as a Route Toward Novel Energetic Materials Using First Principles Crystal Structure Prediction[1]

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At high pressures the underlying chemical bonding in materials can change compared to ambient pressure. This can result in stochiometric changes and novel compounds that are otherwise unstable at ambient pressure. For energetic materials, it is one possible route towards synthesis of high-energy high-density materials, extended solids, as well as energetic salts that more stable at high pressure than ambient pressure. In this talk I will discuss our recent discovery of alkali pentazolates at high pressures consisting of high energy all-nitrogen 5-membered rings (cyclo-N5-). I will also talk about other interesting high-energy materials predicted to exist at high-pressures using first-principles crystal structure prediction. I will discuss the method of crystal structure prediction including its successes, limitations, and challenges when attempting to guide experimental synthesis. I will also discuss more recent results on novel high energy materials at high pressures to motivate future areas of research in this field.

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