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Stable Xenon Nitride at High Pressures YUNWEI ZHANG, FENG PENG, YANMING MA, State Key Lab of Superhard Materials, Jilin University — Nitrogen is the most abundant element on Earth and exists as inert N_2 molecules in the atmosphere. Noble gas nitrides are missing in nature because N_2 molecules do not interact with noble gases at ambient conditions, greatly impeding the understanding of physics and chemistry of such nitrides. We report here a pressure-induced chemical reaction of N_2 with xenon predicted using a swarm-structure searching calculation as implemented in the CALYPSO code [1-2]. This reaction leads to the formation of a hitherto unexpected Xe nitride at megabar pressure accessible to high-pressure experiments. The high-pressure phase with a hypervalent state of Xe by accepting unprecedented Xe-N covalent bonds appears to be the most stable stoichiometry. The Xe bonding situation in this new phase is substantially different from earlier high-pressure examples of ionic Xe bonding or van der Waals interactions.

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Yunwei Zhang
State Key Lab of Superhard Materials, Jilin University

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