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Unrevealing transition mechanism: novel carbons, metallic germaniums, and low-temperature galliums DANIELE SELLI, IGOR A. BABURIN, Technische Universität Dresden, ROMAN MARTONÁK, Comenius University, STEFANO LEONI, Technische Universität Dresden — The quest for novel carbon-based materials is a topic of high priority. Using accelerated molecular dynamics techniques we investigated low-temperature compression of graphite into novel carbon modifications with odd-even topological pattern. At room temperature germanium modifications shows semiconducting properties, while metallicity and superconductivity have been found, so far, only in high pressure modifications. By means of different theoretical methodology, we are able to predict new semiconducting and low pressure metallic Ge phases together with a clearer picture of particular transformation paths and specific indication of possible synthesizabilities. Gallium is among the most challenging elements of the periodic systems. Its polymorphs are structurally very peculiar, characterized by unusual open ground-state crystal structures. While high-pressure promotes close-packed galliums, low-temperature, and the use of mild oxidative chemical approaches, is a way of affecting nucleation patterns towards novel open, clathrate-like compounds.

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