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Novel Si networks in Ca/Si phase diagram under pressure¹ GUOYING GAO, NEIL ASHCROFT, ROALD HOFFMANN, Cornell University — In the Ca/Si phase diagram, many compositions are known. In these calcium silicides, silicon atoms form many different organizations, for example, at low pressure silicons are isolated silicon atoms in Ca_2Si , Si chains in CaSi and corrugated hexagonal Si layers and a three-dimensional network of sp^2 bonds in CaSi_2 . The crystal structures for these silicides under pressure have not been studied completely, and we are very interested in the new chemical and physical behavior of Si in these silicides under pressure. Therefore, we take a theoretical study of Ca_2Si , CaSi and CaSi_2 under pressure. We predicted many interesting Si networks in the calcium silicides under pressure. Si atoms form Si chains in Ca_2Si , flat quadrangular and hexagonal Si layers in CaSi , and 6-coordinated Si tetrahedrons and 4, 8-coordinated Si octahedrons in CaSi_2 at high pressure. All of these predicted structures are dynamically stable. Moreover, these calcium silicides are all metals. Some of them are good candidates to be superconductors.

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