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Theoretical study on possible structures for crystalline silicon dicarbide

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<p>Si, C and SiC are very well known technologically important materials. They have been extensively studied in their multitude of structures and polytypes, but there is a surprising dearth of information for off-50:50 compounds involving Si and C. What are the possible stable structures for such compounds? Using ab initio techniques, we investigate two proposed structures for crystalline SiC₂: cubic pyrite and a tetragonal glitter structure. We find both structures to be metallic and mechanically stable. From their elastic properties, we make an assessment of the hardness of both structures. We find the tetragonal glitter phase to be lowest in energy with a pressure transition from the glitter to pyrite phase at 24.7 GPa.

Level (Hons, MSc,
   PhD, other)?

Phd

Consider for a student
   award (Yes / No)?

Yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

No

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