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Multimillion-atom Reactive Molecular Dynamics Simulations on Oxidation of SiC Nanoparticles[1] YING LI, NICHOLS ROMERO, Argonne National Laboratory, ARGONNE NATIONAL LABORATORY COLLABORATION, UNIVERSITY OF SOUTHERN CALIFORNIA COLLABORATION, KUMAMOTO UNIVERSITY, JAPAN COLLABORATION — High-temperature oxidation of silicon-carbide nanoparticles (nSiC) underlies a wide range of technologies from high-power electronic switches for efficient electrical grid and thermal protection of space vehicles to self-healing ceramic nanocomposites. Here, multimillion-atom reactive molecular dynamics simulations validated by ab initio quantum molecular dynamics simulations predict unexpected condensation of large graphene flakes during high-temperature oxidation of nSiC. Initial oxidation produces a molten silica shell that acts as an autocatalytic 'nanoreactor' by actively transporting oxygen reactants while protecting the nanocarbon product from harsh oxidizing environment. Percolation transition produces porous nanocarbon with fractal geometry, which consists of mostly sp2 carbons with pentagonal and heptagonal defects. This work suggests a simple synthetic pathway to high surface-area, low-density nanocarbon with numerous energy, biomedical and mechanical-metamaterial applications, including the reinforcement of self-healing composites.

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