

Abstract Submitted
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Silicene Catalyzed Reduction of Nitrobenzene to Aniline: a Computational Study CHRISTOPHER MORRISSEY, HAIYING HE, Valparaiso Univ — The reduction of nitrobenzene to aniline has a broad range of applications in the production of rubbers, dyes, agrochemicals, and pharmaceuticals. Currently, use of metal catalysts is the most popular method of performing this reaction on a large scale. These metal catalysts usually require high-temperature and/or high-pressure reaction conditions, and produce hazardous chemicals. This has led to a call for more environmentally friendly nonmetal catalysts. Recent studies suggest that silicene, the recently discovered silicon counterpart of graphene, could potentially work as a nonmetal catalyst due to its unique electronic property and strong interactions with molecules containing nitrogen and oxygen. In this computational study, we have investigated the plausibility of using silicene as a catalyst for the reduction of nitrobenzene. Possible reaction mechanisms will be discussed with a highlight of the difference between silicene and metal catalysts. . All calculations were performed in the framework of density functional theory.

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