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Mechanochemical synthesis of nitridated of zero valent iron for reductive dechlorination

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The widespread application of zerovalent iron (ZVI) in water treatment and remediation has motivated research into modifications of the material that result in improved performance. The newest and most promising involves nitridation, but available methods for nitridation are not environmentally sustainable processes. Here, we demonstrate that mechanochemical molten-salt assisted synthesis can be an effective method to produce surface-nitridated ZVI (SN-ZVI) by replacing the intrinsic FeO_x shell with an iron nitride layer. This modification promoted the dechlorination rate of ZVI by up to 82-fold towards the chlorinated ethenes and chloroform. Enhanced conductivity of the nitridated shell boosts outward electron transfer from the iron core, while the exposed iron nitrides are efficient in activating the C–Cl bond of both trichloroethene and chloroform, and facilitate electron transfer mediated C–Cl cleavage with an energy barrier of 0.20 eV, lower than that of iron oxides (0.78 eV). More importantly, SN-ZVI minimizes the side hydrogen evolution and also promotes deep dechlorination, thus preventing the formation of any toxic chlorinated intermediates, even in the case of highly chlorinated carbons such as tetrachloroethene and chloroform. SN-ZVI maintains its dechlorination performance even after 100 days of water aging, highlighting its great potential for field remediation applications.