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# Molecular dynamics simulation of combustion behavior of coated aluminum hydride nanoparticles in the oxygenated medium: Effects of adding the ethanol atomic coating

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## Abstract

This study used molecular dynamics (MD) simulations to investigate the coated aluminum hydride nanoparticles' thermal, and combustion behavior in an oxygenated medium. Thermal and combustion manner in the presence of two ethanol and nickel atomic coatings were studied. The system's thermal and combustion manners were studied by temperature changes, potential energy changes, penetrated oxygen, heat flux changes, and radial distribution functions. The penetrated atoms showed the combustion process. The greater number of oxygen atoms penetrated, showed the improvement in the combustion process occurred in a shorter time. The results showed that the duration of combustion process in the presence of ethanol atomic coating occurred in a shorter time than nickel atomic coating. Furthermore, the flowing heat flux, and the number of oxygen atoms penetrating atomic structure were higher in the ethanol-coated structure. Therefore, ethanol atomic coating showed better thermal, and combustion behavior. Then, combustion process was studied by adding the percentage of ethanol atomic coating to 12%. By increasing atomic percentage of ethanol coating to 12%, heat flux and number of oxygen penetrated increased from 3.88 to 172 to 7.01 W/m<sup>2</sup> and 225, respectively. Finally, radial distribution function showed that increasing the coating percentage increased number of infiltrated oxygen atoms.