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**Plane wave density functional molecular dynamics study of exothermic reactions of Al/CuO thermites** SULEIMAN OLORIEGBE, THOMAS SEWELL, Department of Chemistry, University of Missouri, Columbia, MO 65211, USA, ZHEN CHEN, SHAN JIANG, Department of Civil and Environmental Engineering, University of Missouri, Columbia, MO 65211, USA, YONG GAN, Department of Engineering Mechanics, Zhejiang University, Hangzhou, Zhejiang 310027, China — Exothermic reactions between nanosize aluminum (Al) and copper oxide (CuO) structures are of current interest because of their high reaction enthalpy and energy density which exceed those of traditional monomolecular energetic compounds such as TNT, RDX, and HMX. In this work, molecular dynamics simulations with forces obtained from plane wave density functional theory are used to investigate the atomic-scale and electronic processes that occur during the fast thermite reactions between Al and CuO nanostructures under adiabatic conditions. Aluminum surfaces in contact with O-exposed and Cu-exposed CuO surfaces are studied. Starting from initial temperature  $T = 800$  K, we have observed: faster chemical reaction at the oxygen-rich interface during the initial 0.5 ps, linear temperature rise, and fast oxygen diffusion into the Al region with the rate  $1.87 \times 10^{-3} \text{ cm}^2/\text{s}$ . The density-derived electrostatic and chemical method is used to evaluate the net atomic charges and charge transfer during the important redox processes. High charge density around the oxygen-exposed interface may be responsible for the faster initial reactions at that interface. The overall reaction rate, determined using the time evolution of Cu-O charge orbital overlap population, is approximately first order.

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