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Cr based Alloy Cr-Y-Mo-W Oxidation Study from First Principals Molecular Dynamics Simulation LEI ZHAO, SHIZHONG YANG, EBRAHIM KHOSRAVI, Southern University and A&M College, SHENGMIN GAO, Louisiana State University — First principles molecular dynamics simulations have been performed to study the stability and oxidation progress of Cr based alloys at high temperatures. The bulk phase of cubic Cr-based alloys is investigated with density functional theory (DFT) calculations and *ab initio* molecule dynamic (MD) method. Diffusion of oxygen atoms within different densities of Y, Mo, and W doping and temperatures in Cr-Y systems is studied in this research. The effects of Y, Mo, and W doping are also studied. The properties of the optimized Y, Mo, and W co-doped Cr-based alloys also studied by using *ab initio* MD method. Further improvement of the oxidation resistance and surface corrosion of Cr-based alloys will be discussed.

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