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Large-scale high-throughput computer-aided discovery of advanced materials using cloud computing TIMUR BAZHIROV, MOHAMMAD MOHAMMADI, Exabyte Inc., KEVIN DING, SERGEY BARABASH, Intermolecular Inc. — Recent advances in cloud computing made it possible to access large-scale computational resources completely on-demand in a rapid and efficient manner. When combined with high fidelity simulations, they serve as an alternative pathway to enable computational discovery and design of new materials through large-scale high-throughput screening. Here, we present a case study for a cloud platform implemented at Exabyte Inc. We perform calculations to screen lightweight ternary alloys for thermodynamic stability. Due to the lack of experimental data for most such systems, we rely on theoretical approaches based on first-principle pseudopotential density functional theory. We calculate the formation energies for a set of ternary compounds approximated by special quasirandom structures. During an example run we were able to scale to 10,656 CPUs within 7 minutes from the start, and obtain results for 296 compounds within 38 hours. The results indicate that the ultimate formation enthalpy of ternary systems can be negative for some of lightweight alloys, including Li and Mg compounds. We conclude that compared to traditional capital-intensive approach that requires in on-premises hardware resources, cloud computing is agile and cost-effective, yet scalable and delivers similar performance.

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