MATERIALS CLOUD, A PLATFORM FOR OPEN MATERIALS SCIENCE

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Materials Cloud is a web platform designed to enable seamless sharing of resources in computational materials science. This includes educational materials, interactive tools, virtual hardware and, in particular, the full provenance of materials science calculations. Through its rich web interface, users can run complex calculations and browse their provenance without domain expertise, while maintaining fine-grained access to the underlying workflows and data.

Materials Cloud is powered by AiiDA [1], a python framework for managing materials science calculations. AiiDA records the data trail leading from the inputs to the results of a computational workflow, and stores it in a local database. Sharing an AiiDA database on Materials Cloud thus provides access to not only the final results of the calculations, but to every step along the way. The data is stored in a persistent and citable way (DOIs). Peers can inspect and download individual files or the whole database, and start their research right from where the original author left off. Further features include lightweight web apps that integrate with AiiDA to run and manage simulations in the cloud.

Materials Cloud is currently in public beta (beta.materialscloud.org), while we add content from our scientific partners and streamline the submission process. The switch to production is planned for the first quarter of 2018. In the medium term, CSCS is developing a stack of federated services for authentication and authorization, object storage and web services, to be extended to CINECA (Italy) and Jülich (Germany) to build a decentralized cloud.

[1] G. Pizzi et al., Comp. Mat. Sci. 111, 218 (2016) - www.aiida.net