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Total Energy and Forces in Africa

Abstract:

Despite the scarcity of computational power in Africa, some research and training in the calculation of the electronic structure of different systems are ongoing. This talk will highlight the work of researchers in certain regions of Africa as well as showcase some successful training efforts and collaborations in the computational determination of total energy and forces of various systems. Collaborations are important in Africa as there is only a small percentage of researchers who can carry out high-level calculations of large systems without linking up with groups outside their home countries. At the East Africa Institute for Fundamental Research (EAIFR), which is an ICTP Partner Institute, we are teaming up with others to create infrastructure for such high-level calculations as well as developing methods that can be used to carry out calculations on large systems with the accuracy of high-level first-principles approaches. At the same time, we are building human capacity that can make significant impact in Africa using these infrastructure and methods. Some of our work at EAIFR on determining the excited states of large quantum dots, with more than 10,000 electrons, will also be presented.

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