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Improving usability of DFT codes by using GUI software C-Tools

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We develop GUI software C-Tools [1] to improve the usability of DFT codes for materials. There are a variety of DFT codes with each strength, and to combine the strength we have to transfer among the codes. For this purpose, we have developed an input format conversion system, named as C-Tools, with a developed unified input format in XML as a common interlanguage among various formats. C-Tools can convert the input files between different codes and can generate an input file from a structure file for a material. The input files can be easily created by clicking the [load] and [save] button. Now C-Tools supports the five file formats for DFT codes, xTAPP [2], OpenMX [3], RSDFT [4], VASP [5], and Quantum ESPRESSO (PWscf) [6]. We can use C-Tools for performance analysis of DFT codes in HPCI system. We show the results in K computer.

[1] http://ma.cms-initiative.jp/en/application-list/tapioca.
[2] Yoshihide Yoshimoto, TAPP consortium tapp@cms.phys.s.u-tokyo.ac.jp.
[3] T. Ozaki, H. Kino, J. Yu, M.J. Han, N. Kobayashi, M. Ohfuti, F. Ishii, T. Ohwaki, H.Weng, Computer code OpenMX. http://www.openmx-square.org/.
[4] J.-I. Iwata, D. Takahashi, A. Oshiyama, B. Boku, K. Shiraishi, S. Okada, and K. Yabana, J. Comput. Phys. 229, 2339 (2010).; http://ma.cms-initiative.jp/ja/listapps/rsdft/.
[5] http://www.vasp.at.
[6] http://www.quantum-espresso.org.

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