

Erratum: “DFTB+, a software package for efficient approximate density functional theory based atomistic simulations” [J. Chem. Phys. 152, 124101 (2020)]

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The implementation of the GPU support in DFTB+, as described in Sec. III C of the original publication,¹ was developed based on a previous unpublished implementation by Jacek Jakowski. In order to acknowledge his work on this first implementation, the authors of the original publication wish to include J. Jakowski as co-author. The scientific content of the original publication is not affected.

REFERENCE

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