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Abstract Submitted
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New DMFT capabilities in CASTEP[1] EVGENY PLEKHANOV, Department of Physics, Faculty of Natural and Mathematical Sciences King's College London Strand, London, WC2R 2LS, UK, VINCENT SACKSTEDER, Department of Physics, Royal Holloway University of London, Egham, Surrey TW20 0EX, UK, PHIL HASNIP, MATT PROBERT, Department of Physics, University of York, Heslington, York YO10 5DD, UK, STEWART CLARK, Department of Physics, University of Durham, Durham DH1 3LE, UK, CEDRIC WEBER, Department of Physics, Faculty of Natural and Mathematical Sciences King's College London Strand, London, WC2R 2LS, UK, KEITH REFSON, Department of Physics, Royal Holloway University of London, Egham, Surrey TW20 0EX, UK — We present the first implementation of Dynamical Mean-Field Theory in UK's major ab-initio code CASTEP [1]. This implementation: i) is modular; ii) allows great flexibility in choosing local basis set for downfolding/upfolding of self-energy; iii) permits wide choice of impurity solvers (including external solver libraries); and iv) gives the user a possibility to use several self-consistency schemes and calculate total energy and forces. We explain in details the theoretical framework used. We benchmark our implementation on several strongly-correlated insulating systems with d- and f-shells: γ-Ce and Ce_2O_3 by using Hubbard I and CTHYB-QMC solvers. Our results appear to be in excellent agreement with the reference data published previously in the literature [2,3,4]. [1] E. Plekhanov, et al. in preparation (2016). [2] L. Pourovskii, et al. Phys. Rev. B 76, 235101 (2007). [3] B. Amadon, et al. Phys. Rev. B 77, 205112 (2008). [4] J. Kune, et al. Phys. Rev. Lett. 99, 156404 (2007).

[1]EPSRC-funded project "Strong Correlation meets Materials Modelling: DMFT and GW in CASTEP"

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