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Order-N Electronic Total Energy Package

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References

1. Prentice JCA, Aarons J, Womack JC, Allen AEA, Andrinopoulos L, Anton L, Bell RA, Bhandari A, Bramley GA, Charlton RJ, Clements RJ, Cole DJ, Constantinescu G, Corsetti F, Dubois SMM, Duff KKB, Escartín JM, Greco A, Hill Q, Lee LP, Linscott E, O'Regan DD, Phipps MJS, Ratcliff LE, Serrano AR, Tait EW, Teobaldi G, Vitale V, Yeung N, Zuehlsdorff TJ, Dziedzic J, Haynes PD, Hine NDM, Mostofi AA, Payne MC, Skylaris CK(06/05/2020) , https://pubs.aip.org/aip/jcp/article/152/17/174111/198202/The-ONETEP-linear-scaling-density-functional, https://pubs.aip.org/aip/jcp/article/152/17/174111/198202/The-ONETEP-linear-scaling-density-functional, 152, 174111

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