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R. Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalleri, S. Casassa, L. Maschio, M. Ferrabone, M. De la Pierre, Ph. D'Arco, Y. Noël, M. Causà, M. Rèrat, and B. Kirtman, CRYSTAL14: A Program for the Ab initio Investigation of Crystalline Solids Int. J. Quantum Chem., 2014, 114, 1287-1317

(see the www.crystal.unito.it web site for updated citations)

- 8. To refer to specific options and technical details of the CRYSTAL14 implementation please quote:
  - R. Dovesi, V.R. Saunders C. Roetti, R. Orlando, C.M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M.



Harrison, I.J. Bush, Ph. D'Arco, M. Llunell, M. Causà, Y. Noël CRYSTAL14 User's Manual, University of Torino, Torino, 2014

9. References to specific algorithms as implemented in CRYSTAL14 can be found at <a href="http://www.crystal.unito.it">http://www.crystal.unito.it</a> under the "Theoretical background" section.

It would be appreciated if a copy of such publications were sent to one of the authors.

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