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Part 1: CRYSTAL23 License agreement

In the following,

- the term "the authors", is to be construed as meaning as the names as listed in the CRYSTAL23 User's Manual: *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. Noel, L. Maschio, A. Erba, M. Rérat, S. Casassa, B.G. Searle, J.K. Desmarais*
- the term "the managing authors" identifies the authors of CRYSTAL23 affiliated to the Theoretical Chemistry Group at the Department of Chemistry of the University of Torino, responsible for the maintenance, support, distribution, documentation, development and general management of the software: *S. Casassa, B. Civalleri, J. K. Desmarais, A. Erba, L. Maschio*
- the term "I" is referred to you as the end user licensee (Research Group leader) and "registered address" corresponds to the address of the end user licensee as specified during the registration process.

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*A. Erba, J. K. Desmarais, S. Casassa, B. Civalleri, L. Donà, I. J. Bush, B. Searle, L. Maschio, L.-E. Daga, A. Cossard, C. Ribaldone, E. Ascrizzi, N. L. Marana, J.-P. Flament, B. Kirtman "CRYSTAL23: A Program for Computational Solid State Physics and Chemistry" J. Chem. Theory Comput. 2023, 19, 6891–6932.
<https://doi.org/10.1021/acs.jctc.2c00958>*

9. I understand that when using specific options of CRYSTAL23 I am invited to cite the relevant publications as found in the *CRYSTAL23 User's Manual* or/and in the CRYSTAL23 output file.

10. I understand that when referring to specific keywords and technical details of the CRYSTAL23 implementation I am invited to cite:

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. Noel, L. Maschio, A. Erba, M. Rérat, S. Casassa, B.G. Searle, J.K. Desmarais "CRYSTAL23 User's Manual", University of Torino, Torino, 2023

11. I understand that no large program such as CRYSTAL23 can be considered to be bug free, and accordingly the authors supply the software on an "as is" basis, with no additional responsibility or liability or warranty of merchantability or fitness for a particular purpose.

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- iii. CRYSTAL23 for Windows is supplied as a self-installing file and a Graphical User Interface.
- iv. Precompiled executables include sequential (crystal, properties, crystalOMP) and replicated data parallel versions (Pcrystal, Pproperties, PcrystalOMP). The massively-parallel versions (MPPcrystal, MPPcrystalOMP) are only supplied as object files.
- v. A web-based tool, CRYSPLOT, is freely available to visualize and plot properties computed with CRYSTAL (<http://crysplot.crystalsolutions.eu>). If you use it and make plots to be included in any publication please cite:

G. Beata, G. Perego and B. Civalleri "CRYSPLOT: A New Tool to Visualize Physical and Chemical Properties of Molecules, Polymers, Surfaces, and Crystalline Solids" J. Comput. Chem. 40 (2019) 2329-2338

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Aethia S.r.l. is available to answer any question submitted by email to the email address info@crystalsolutions.eu ^[1]_[SEP]