A View from Academia: the Longest-term Perspective?

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The ONETEP code [1] is a software package that enables large-scale first-principles electronic structure calculations of real materials as a result of some distinctive features including the *in situ* optimisation of a set of local orbitals in terms of a basis set equivalent to a set of plane-waves. This talk will reflect on the experience of engagement with industry at an unusually early stage of development, including an element of co-design of functionality to meet the needs of industrial users that evolved into a partnership that has lasted over 15 years.

REFERENCES

[1] J. C. A. Prentice, J. Aarons, J. C. Womack, A. E. A. Allen, L. Andrinopoulos, L. Anton, R. A. Bell, A. Bhandari, G. A. Bramley, R. J. Charlton, R. J. Clements, D. J. Cole, G. Constantinescu, F. Corsetti, S. M.-M. Dubois, K. K. B. Duff, J. M. Escartín, A. Greco, Q. Hill, L. P. Lee, E. Linscott, D. D. O'Regan, M. J. S. Phipps, L. E. Ratcliff, Á. Ruiz Serrano, E. W. Tait, G. Teobaldi, V. Vitale, N. Yeung, T. J. Zuehlsdorff, J. Dziedzic, P. D. Haynes, N. D. M. Hine, A. A. Mostofi, M. C. Payne, C.-K. Skylaris. The ONETEP linear-scaling density functional theory program. J. Chem. Phys. 152, 174111 (2020). DOI: 10.1063/5.0004445