APPLICATIONS IN MOLECULAR PHYSICS OF A BASIS IN THE SPACE OF PRODUCTS

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Previously we showed that our method [1] of basis set reduction allows relatively straightforward calculation of molecular spectra from the Petersilka-Gossmann-Gross equations [2].

Here we give further examples from molecular physics where our method simplifies and accelerates computations, building on data imported from the siesta code.

References:
[1] Foerster D, J. Chem. Phys. 128 034108 (2008) and P. Koval and D. Foerster, arXiv:0904.3834v1 (2009)

[2] Petersilka M, Gossmann U J and Gross E K U, Phys. Rev. Lett. 76 1212 (1996)