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Structure Determination of a new Molecular White-Light Source

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The molecular structure of the white light generating amorphous material [(PhSn)4S6] is investigated using X-ray scattering coupled with a rigid molecular Reverse-Monte-Carlo (RMC) modeling approach. Experimental proof for an adamantane-like molecule structure is found. The intermediate-range structure is analysed, indicating a strong preference for distinct cluster orientations. It is shown that rigid molecular RMC simulations are feasible for structure analysis without using potential-related features. [1-3]

Literature

- [1] N. W. Rosemann, J. P. Eußner, E. Dornsiepen, S. Chatterjee, S. Dehnen, Organotetrel Chalcogenide Clusters: Between Strong Second-Harmonic and White-Light Continuum Generation, *Journal of the American Chemical Society* **138**(50), 16224-16227 (2016).
- [2] N. W. Rosemann, J.P. Eußner, A. Beyer, S. W. Koch, K. Volz, S. Dehnen, S. Chatterjee, A highly efficient directional molecular white-light emitter driven by a continuous-wave laser diode, *Science* **352**(6291), 1301-1304 (2016).
- [3] B. D. Klee, E. Dornsiepen, J. R. Stellhorn, B. Paulus, S. Hosokawa, S. Dehnen, W.-C. Pilgrim, Structure Determination of a new Molecular White-Light Source, submitted to *Physica Status Solidi B* in February 2018.

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