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Models of $\mathbf{Ge}_x\mathbf{Se}_{1-x}$[1] MARC-ANDRÉ MALOUIN, NORMAND MOUSSEAU, Departement de physique and RQMP, Universite de Montreal, Montreal (QC), Canada — We present numerical models of chalcogenide glasses constructed using the effective two and three body interaction potential developed by Mauro and Varshneya [1] combined with the activation-relaxation technique (ART nouveau) [2]. Structures are prepared starting from a random distribution, avoiding biases and crystalline remnants. Structural properties are studied mainly via characteristic system measurements including partial and total radial distribution functions, bond angle distributions, mean coordinations and bonds population. Results are shown for Ge_xSe_{1-x} for various x concentrations and compared to both experimental measurements and *ab initio* simulation results.
[1] J.C. Mauro and A.K. Varshneya, J. Am. Ceram. Soc., 89 [7] 2323-6 (2006).
[2] R. Malek and N. Mousseau, Phys. Rev. E 62, 7723 (2000).

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