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Short Range Order Signature in Crystalline and Amorphous GeSbTe Xanes Spectra¹ JEAN-YVES RATY, CÉLINE OTJACQUES, RENGIN PEKOZ, University of Liège, CHRISTOPHE BICHARA, CNRS- University Aix-Marseille, VINCE LORDI, Lawrence Livermore National Laboratory — A new implementation of XANES spectra calculations within DFT and PAW potentials is used to compute the XANES spectra of various amorphous and crystalline GeSbTe structures. A clear correlation between the local order, either tetrahedral or distorted octahedral, and the shape of the XANES signal is observed. These calculations provide a new interpretation of past XANES measurements, relating essentially the phase change mechanism to a moderate modification of the local environment of the Ge atoms.

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