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Simulation of structural and electronic properties of amorphous tungsten oxycarbides KALIAPPAN MUTHUKUMAR, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Electron beam induced deposition with tungsten hexacarbonyl $W(CO)_6$ as precursors leads to granular deposits with varying compositions of tungsten, carbon and oxygen. Depending on the deposition conditions, the deposits are insulating or metallic. We employ an evolutionary algorithm to predict the crystal structures starting from a series of chemical compositions that were determined experimentally. We show that this method leads to better structures than structural relaxation based on guessed initial structures. We approximate the expected amorphous structures by reasonably large unit cells that can accommodate local structural environments that resemble the true amorphous structure. Our predicted structures show an insulator to metal transition close to the experimental composition at which this transition is actually observed. Our predicted structures also allow comparison to experimental electron diffraction patterns.

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