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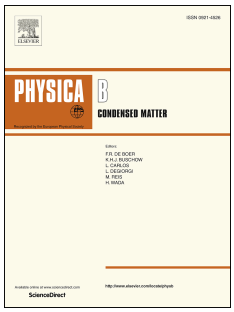

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Effective bandstructures from unfolding supercells with vacancies

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ABSTRACT

We study how vacancies alter the effective primitive cell bands projected out of supercell eigenstates via Brillouin zone unfolding. Two types of vacant primitive cells are of particular interest: Fully vacant, in which all atoms in a single cell are missing; and net fully vacant, in which the atoms comprising a full set for a single cell are missing from more than one cell. We find that a fully vacant primitive cell and a net fully vacant primitive cell have the same effect on the primitive cell bands. We show that the probability reduction for any primitive cell band is the same, regardless of band or wavevector in the primitive cell Brillouin zone, for both fully and net fully vacant primitive cells. We illustrate these results with a two-band model.