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**The formation and pinning of folds in two-dimensional materials**
YUANXI WANG, VINCENT CRESPI, Pennsylvania State University — The isolation of two-dimensional materials such as graphene, hexagonal boron nitride and transition metal dichalcogenides from their bulk counterparts allows a new kind of crystal defect - a fold. Using density functional theory simulations, we characterize the geometry, energetics and formation mechanism of different kinds of folds in fluorinated graphene and modified molybdenum disulfide sheets with sulfur vacancies and selenium substitutions. Furthermore we demonstrate two methods of pinning a fold once it is formed: by the preferential adsorption of adatoms along the fold-line, or by forcing the registry of the folded sheets via selective p- or n-type doping. The latter can be applied to the design and self-assembly of two-dimensional sheets into more complex geometries.

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