

Abstract Submitted
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Band Parameters of Two-Dimensional Materials: Phosphorene and Silicene LOK LEW YAN VOON, The Citadel, ALEJANDRO LOPEZ BEZANILLA, Argonne National Lab, JIANWEI WANG, YONG ZHANG, U North Carolina Charlotte, MORTEN WILLATZEN, Technical University Denmark, THE CITADEL COLLABORATION, ANL COLLABORATION, UNCC COLLABORATION, DTU COLLABORATION — The method of invariant is used to derive effective Hamiltonians in the presence of strain and external fields for phosphorene and silicene as examples of two-dimensional materials with and without a band gap. The band structure parameters have been obtained by fitting to density-functional theory calculations.

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