



## Computational Materials Design for Band Gap Engineering

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Deadline for manuscript  
submissions:

**closed (30 August 2019)**

### Message from the Guest Editor

Band gap engineering is an attractive area for computational materials design, and addresses the control of multiscale material features to achieve superior optical, thermal, and electronic properties. This Special Issue considers all manuscripts addressing the band gap design of crystalline materials (0d, 1D, 2D, 3D) in multiple length scales and multiple material models for a wide range of applications in energy, electronics, optoelectronics, biomedical, and aerospace industries. The current Special Issue covers all manuscripts utilizing first-principles computations, atomistic simulations, and meso-, macro-, and multi-scale algorithms to understand and design band gap in all crystalline materials, including multifunctional nanomaterials, metamaterials, heterostructures, and interfaces. We welcome all submissions from all studies dealing with computational approaches for band gap engineering.





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## Message from the Editor-in-Chief

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