Electronic supplementary information:

Computational prediction of a novel 1D InSeI nanochain with high stability and promising wide-bandgap properties

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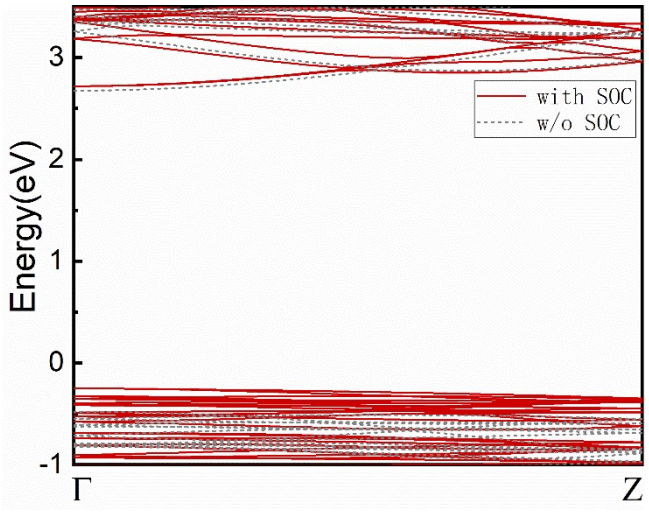

Figure S1. Band structures of InSeI single nanochain calculated by HSE06 with SOC (in red) and without SOC (in grey), respectively.

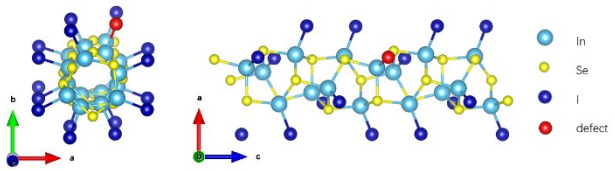

Figure S2. Structural configuration of 1D single nanochain of InSeI with a surface defect of I vacancy (in red).

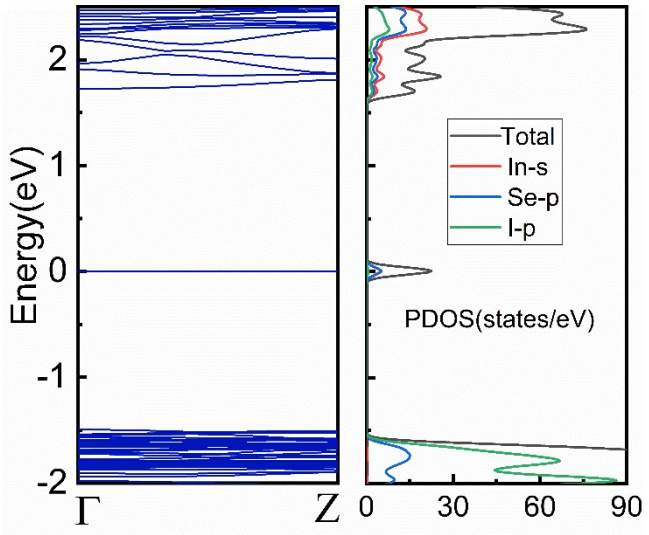

Figure S3. Band structure and the partial density of states (PDOS) calculated by HSE06 of InSeI singe nanochain with a surface defect of I vacancy.