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Unusual Optoelectronic Properties of Hydrogenated Bilayer Silicene: From Solar Absorber to Light-emitting Diode Applications[1] BING HUANG, National Renewable Energy Laboratory, HUI-XIONG DENG, Institute of Semiconductors, Chinese Academy of Sciences, HOONKYUNG LEE, School of Physics, Konkuk University, CHANGWON PARK, MINA YOON, BOBBY SUMPTER, CNMS, Oak Ridge National Laboratory, FENG LIU, Department of Materials Science and Engineering, University of Utah, SEAN SMITH, Chemical Sciences Division, Oak Ridge National Laboratory, SU-HUAI WEI, National Renewable Energy Laboratory — Silicon is arguably the greatest electronic material, but not so good an optoelectronic material. By employing first-principles calculations and cluster-expansion approach, we discover that hydrogenated bilayer silicene (BS) shows promising potential as new optoelectronic materials. Most significantly, hydrogenation will covert the intrinsic BS, a strongly indirect semiconductor, into a direct-gap semiconductor with a widely tunable band gap. At low hydrogen concentrations, four ground states of single- and double-side hydrogenated BS are characterized with dipole-allowed direct (or quasidirect) band gaps in the desirable range from 1 to 1.5 eV, suitable for solar applications. At high hydrogen concentrations, three well-ordered double-side hydrogenated BS structures exhibit direct (or quasidirect) band gaps in the range of red, green, and blue colors, respectively, affording white light emitting diodes. Our findings open a door to the search of new silicon-based light-absorption and light-emitting materials for earth-abundant high-efficiency optoelectronic applications.

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