**Electronic Supplementary Information (ESI)**

# Electronic structure and optical properties of novel monolayer gallium nitride and boron phosphide heterobilayer

A. Mogulkoc*
*Department of Physics, Faculty of Sciences, Ankara University, 06100, Tandogan, Ankara, Turkey*

Y. Mogulkoc
*Department of Engineering Physics, Faculty of Engineering,*
*Ankara University, 06100, Tandogan, Ankara, Turkey*

M. Modarresi
*Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran. and*
*Laboratory of Organic Electronics, Department of Science and Technology,*
*Campus Norrköping, Linköping University, SE-60174 Norrköping, Sweden*

B. Alkan
*Department of Engineering Physics, Faculty of Engineering,*
*Ankara University, 06100, Tandogan, Ankara, Turkey*

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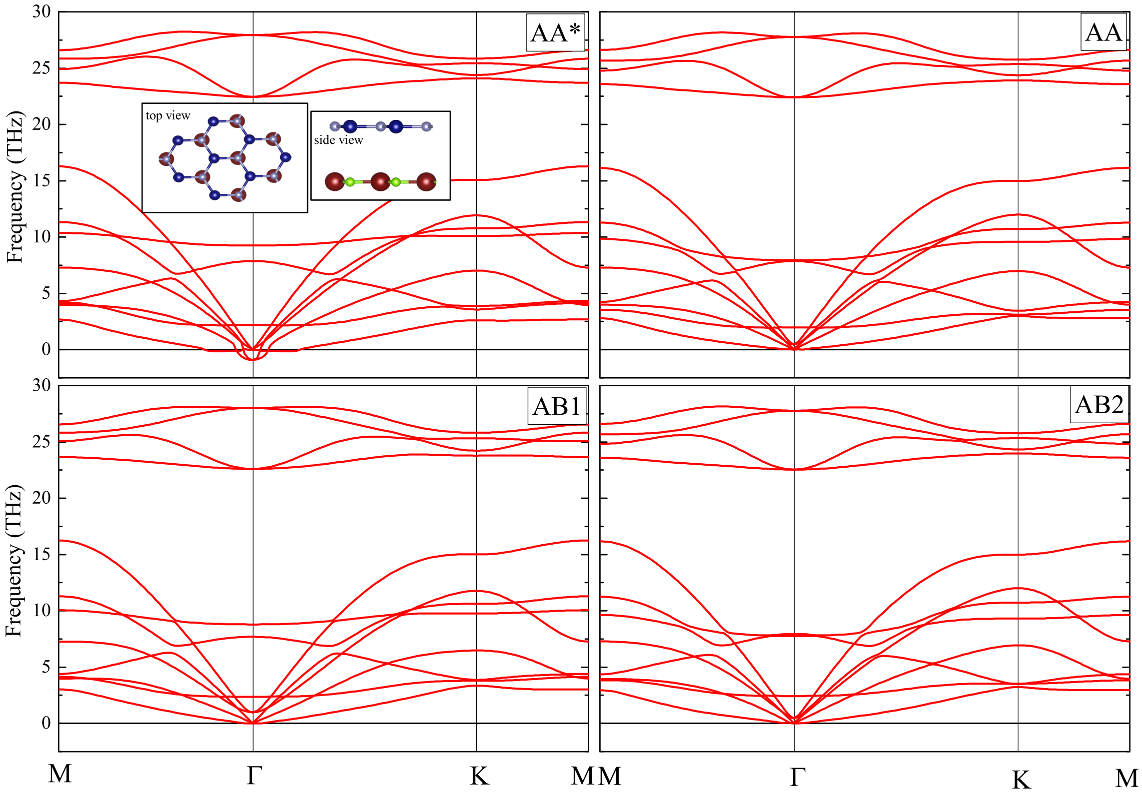

FIG. S1: Phonon spectra of MGaN/MBP heterobilayers.

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*Electronic address: `mogulkoc@science.ankara.edu.tr`

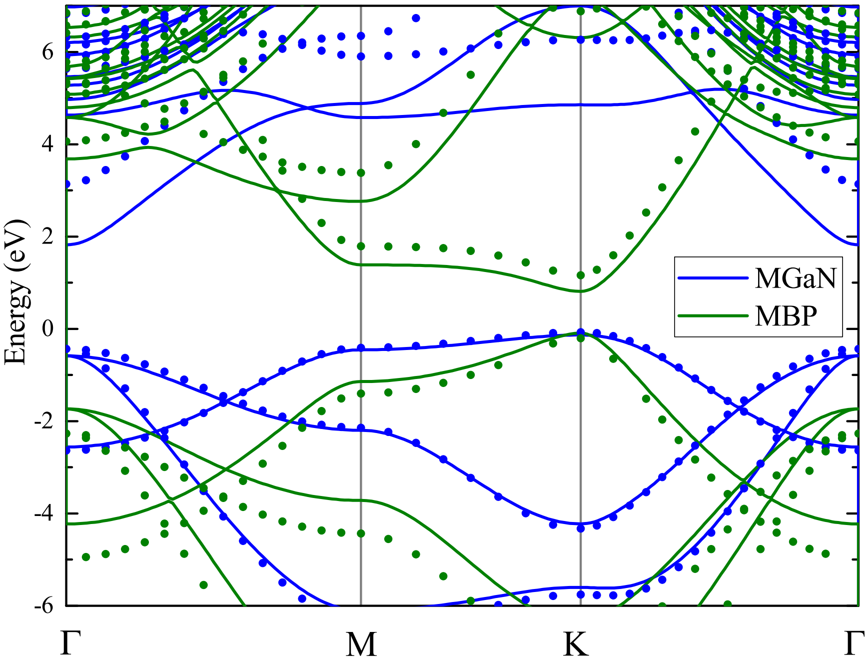

FIG. S2: Energy band spectrum of MGaN and MBP for PBE (solid) and HSE06 (dotted).

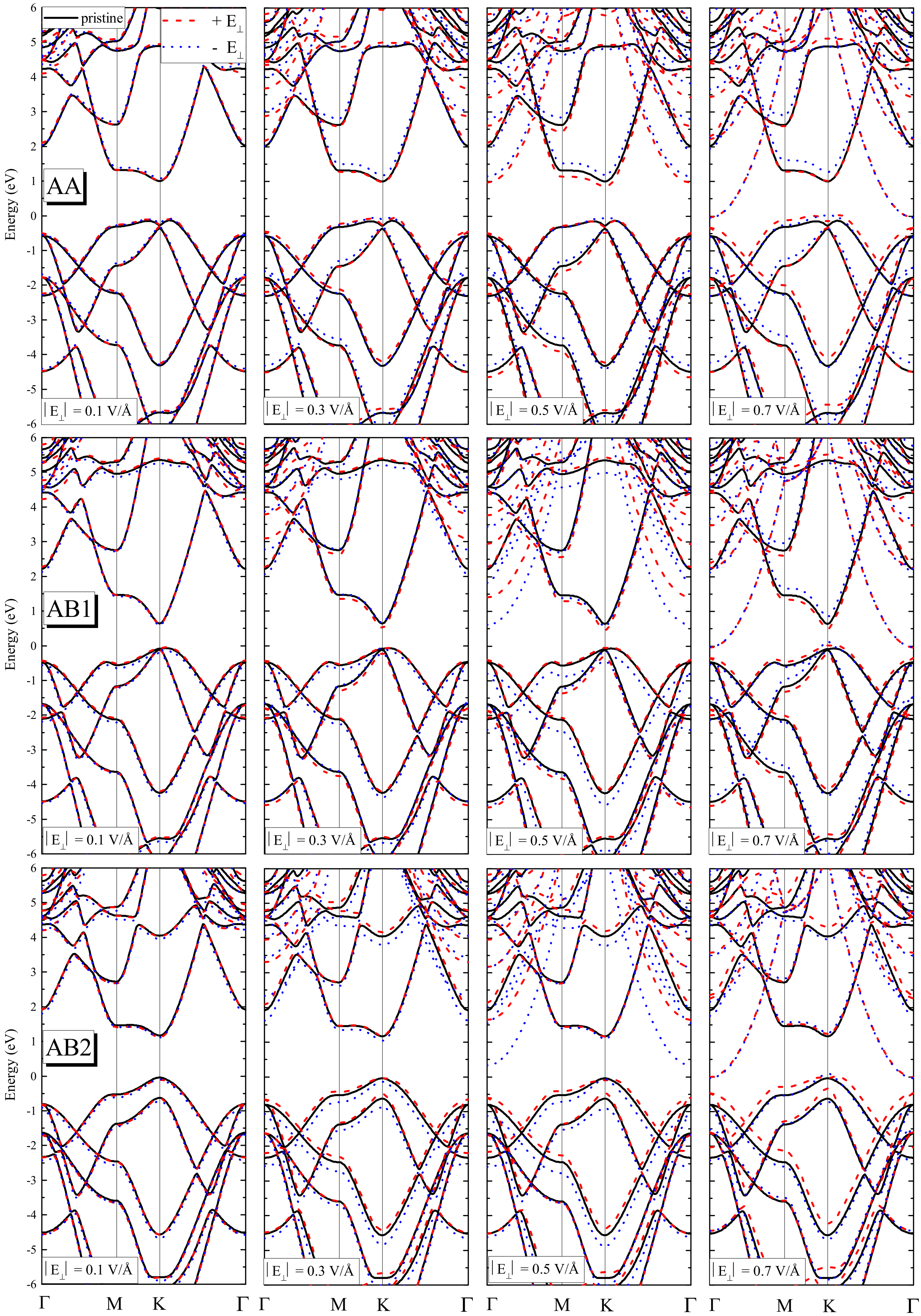

FIG. S3: Electronic band diagram of AA, AB1 and AB2 stack of mGaN/MBP heterobilayers in the presence of perpendicular electric field.