**Presentation Title**

Critical evaluation of various spontaneous polarization models and induced electric fields in III-nitride multi-quantum wells

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**Abstract:**

In this paper, ab initio calculations are used to determine polarization difference in zinc blende (ZB), hexagonal (H) and wurtzite (WZ) AlN-GaN and GaN-InN superlattices. It is shown that a polarization difference exists between WZ nitride compounds, while for H and ZB lattices the results are consistent with zero polarization difference. It is therefore proved that the difference in Berry phase spontaneous polarization for bulk nitrides (AlN, GaN and InN obtained by Bernardini et al. {Phys. Rev. B **1997**, 56, R10024} and Dreyer at al. {Phys. Rev. X **2016**, 6, 021038} was not caused by the different reference phase. These models provided absolute values of the polarization that differed by more than one order of magnitude for the same material, but they provided similar polarization differences between binary compounds, which agree also with our ab initio calculations. In multi-quantum wells (MQWs), the electric fields are generated by the

well-barrier polarization difference, hence the calculated electric fields are similar for the three models, both for GaN/AlN and InN/GaN structures. Including piezoelectric effect, which can account for 50% of the total polarization difference, these theoretical data are in good agreement with photoluminesce measurements in GaN/AlN MQWs. Therefore, the three models considered above are equivalent in the treatment of III-nitride MQWs and can be equally used for the description of the electric properties of active layers in nitride based optoelectronic devices

**Biography of presenting author**

I, Mr. Ashfaq Ahmadl studied Physics at Quaid-I-Azam University Islamabad, Pakistan and did my Master in Physics in 2015.Then I join the Higher Education Department in Pakistan as Lecturer of Physics from 2015 to 2019 . At the end of 2020 I got PhD scholarship in Poland and started my PhD here in the Institute of High Pressure Physics Polish Academy of Sciences Poland. I published two articles in this one year PhD studied.

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