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Strong Second Order Piezoelectric Effect in InGaAs/GaAs Nanostructures[1] GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Laboratory, XIFAN WU, DAVID VANDERBILT, Rutgers University — We show that the piezoelectric effect that describes the emergence of an electric field in response to a crystal deformation has strong contributions in III-V semiconductors such as GaAs and InAs from second-order effects that have been neglected so far. We calculate the first and second-order piezoelectric tensors using density functional theory. Applying these calculated tensors to quantum wells [1] gives piezoelectric fields that agree well with experiments, whereas neglect of non-linearities leads to qualitative disagreements. We find that the linear and the quadratic piezoelectric coefficients have the opposite effect on the field. Which term dominates is stronlgy dependend on concentration x for quantum wells and for large x the quadratic terms strongly dominates. Applying our theory to quantum dots [2] shows that both term nearly cancel each other so neglecting piezoelectricity is a better approximation than using only the linear term. Thus, the piezoelectric field turns out to be a rare example of a physical quantity for which the first-order and second-order contributions are of comparable magnitude.

[1] G. Bester, A. Zunger, X. Wu and D. Vanderbilt, Phys. Rev. B. **74**, 081305(**R**) (2006). [2] G. Bester, X. Wu, D. Vanderbilt and A. Zunger, Phys. Rev. Lett. **96**, 187602 (2006).

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Gabriel Bester
National Renewable Energy Laboratory

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