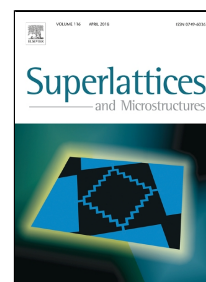


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First-Principles Investigation of Size-Dependent Piezoelectric Properties of Bare ZnO and ZnO/MgO Core-Shell Nanowires

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Abstract:

Using first-principles density functional theory (DFT) calculations, we evaluate and compare the piezoelectric properties in *bare* ZnO and ZnO/MgO *core-shell* nanowires. The study confirms that effective piezoelectric coefficient in bare ZnO nanowires is a highly diameter sensitive parameter. In the thinnest ZnO nanowire, with only one layer of atoms, the effective piezoelectric coefficient attains a maximum value of 12.21 C/m². On the other hand, for the first time, we report that piezoelectricity in MgO-passivated ZnO nanowires exhibits a *lesser* size dependence than in the bare ones, a finding that may prove useful in the design of emerging ultraviolet optoelectronic devices.

Keywords:

ZnO; ZnO/MgO nanowire; DFT calculation; piezoelectric properties; surface passivation

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