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Role of Atomic and Electronic Structure of $LiTaO_3$ and $LiNbO_3$ Piezoelectric for Direct NanoBonding with Si And SiO_2: Comparison of Measured Surface Energies with Computed ΔG and Infra-Red Absorption MOHAMMED SAHAL, ABBIE ELISON, SHEFALI PRAKASH, SRIVATSAN SWAMINATHAN, RILEY RANE, BRIAN BAKER, JACOB KINTZ, ALIYA YANO, SAAKETH NARAYAN, ALEX BRIMHALL, LAUREN PUGLISI, ROBERT CULBERTSON, NICOLE HERBOTS, Arizona State University, Dept. of Physics, PROF. N. HERBOTS NANOBONDING TEAM — Piezoelectric $LiTaO_3$ /$LiNbO_3$/Si hetero-structures have two major issues: mismatch of crystal structure, lattice constants and especially coefficient of thermal expansion, by an order of magnitude. Hence, this work uses NanoBonding^{TM} [1] to directly bond $LiTaO_3$ to Si and $LiNbO_3$ to SiO_2 via Surface Energy Engineering (SEE). SEE modifies in synergy surface hydro-affinity (H-A) and Surface Energy (SE) to far-from-equilibrium states likely to react in air at RT. HA and SE are measured via Three Liquid Contact Angle Analysis in air. SEs are 41 2 mJ/m^2 for $LiTaO_3$ and 39 2.5 mJ/m^2 for $LiNbO_3$, thus close. SE is compared to computed ΔGs of interaction for $LiTaO_3$, -104 mJ/m^2, and $LiNbO_3$, -115 mJ/m^2, in 25% H_R. Thus, ΔGs favor water adsorption with negative values, -104 mJ/m^2 and -115 mJ/m^2 respectively. Negative ΔG can favor spontaneous bonding of $LiTaO_3$ to Si and hydrophobic $LiNbO_3$ to hydrophilic SiO_2. Experimentally, SEE is needed to activate bonding of $LiTaO_3$ to Si, and $LiNbO_3$ to SiO_2. [1] Herbots, et al. U.S. Pat. # 9,018,077 (2015), 9,589,801(2017), pend. (2020)

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