PBE-D3, pob-TZVP, SHRINK 8 8, Bipolar 18 18, TOLINTEG 8 18, XXLGRID, TOLDEE 8 $(0.87 - 0.98)V_{eq}$ and $(0.98 - 1.08)V_{eq}$ -941.125 Calcite I PV) / F.U. (a.u.) Cubic fit Calcite I -941.150 -Calcite II Cubic fit Calcite II -941.175 -941.200Analytic $+E_{ZP}$ + -941.225Intersection P= 1.9874 GPa -941.250 -G = -941.208 a.u.Ш -941.275-941.300 -4 **P** (**GPa**)