First principles exploration of the possibility of high mobility phases and alloys of group IV semiconductors.\textsuperscript{1} JAY SAU, MARVIN COHEN, UC Berkeley and Lawrence Berkeley National Laboratory — At present it is known that in some cases the mobility of Si can be increased through alloying of Si with Ge and straining Si epitaxially. Here we examine the possibility of higher mobility group IV semiconductors. Currently it appears that Ge based devices might become popular in the near future due to the higher mobility of Ge. Using Density Functional Theory and GW quasiparticle corrections together with $k$-$p$ theory and EPM, we examine how strain and alloying Sn can be used to increase the mobility of Ge related semiconductors. In this study we account for alloy scattering due to Sn impurities in Ge using first principles calculations. We find that the effect of alloy scattering is not prohibitively large. Recently CVD based methods [Kouvetakis et al. APL, 81, 2992(2002)] have been developed to fabricate these alloys making such studies of increased technological relevance.

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