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NaAlSi: An Unusual Self-Doped Semimetal With Free Electrons and Covalent Holes HAHNBIDT RHEE, SWAPNONIL BANERJEE, ERIK YLVISAKER, WARREN PICKETT, UC Davis, WARREN PICKETT'S GROUP TEAM — The ternary compound NaAlSi is a layered *sp* conductor that superconducts at a relatively high T_c of 7 K. Using first principles electronic structure calculations (the FPLO code), we find that NaAlSi is a self-doped semimetal with several unusual characteristics (in addition to the interesting fact that its structure is the same as those of the Fe-pnictide 111 coupounds). Na gives up its electron, allowing the Si-Al sublayer to form a distinct set of covalent valence bands, which are nearly filled. A strongly directional, Al-derived free electron band overlaps the valence bands, providing the electron carriers. The k_z dispersion is small, but it occurs at the Fermi level, leading to unusual Fermi surfaces. Wannier functions will be provided to assist in the understanding of the bonding, and comparison with the CaAlSi compound, with one additional electron and a different structure (the MgB_2 structure) will be presented.

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