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Effects of disordered isovalent substitution in Fe-based superconductor[1] LIMIN WANG, TOM BERLIJN, Brookhaven National Laboratory, YAN WANG, University of Florida, CHAI-HUI LIN, Stony Brook University, Brookhaven National Laboratory, P.J. HIRSCHFELD, University of Florida, WEI KU, Brookhaven National Laboratory, Stony Brook University — Using a recently developed first-principles method for disordered materials [1-2], we investigate the effect of isovalent substitution in Fe-based superconductors, $BaFe_2(As_{1-x}P_x)_2$, $FeTe_{1-x}Se_x$, and $Ba(Fe_{1-x}Ru_x)_2As_2$. For anion substitutions (the first two cases) effects of impurity scattering are found mostly in the anion bands. By contrast, the Ru substitution introduces much stronger scattering in the Fe bands. Surprisingly, in all the cases, the pockets near the chemical potential are the least affected, due to the low density of states near the chemical potential. Together, our results suggest an interesting scenario of enhancing superconductivity.

[1] T. Berlijn, D. Volja, W. Ku, Phys. Rev. Lett. 106, 077005 (2011).
[2] W.Ku, T. Berlijn, CC. Lee, Phys. Rev. Lett. 104, 216401 (2010).

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Limin Wang
Brookhaven National Laboratory

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