



Calculated natural band offsets of all II–VI and III–V semiconductors: Chemical trends and the role of cation d orbitals

[Gi !<i U\]K Y\]UbX'5'YI 'Ni b\[Yf'](#)

[7 \]U\]cb. '5dd' \]YX'D\mg\]Mg' @YHfg'72Z &\\$%f% - , t/Xc\]. %\\$"%\\$*' #/%&%&\(-](#)

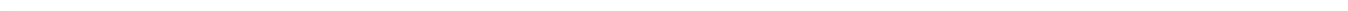
[J \]Yk 'cb\]bY. \hnd. #Xl "Xc\]"cf\[#/\\$"%\\$*' #/%&%&\(-](#)

[J \]Yk 'HUV'Y'cZ7 cbH/bfg. \hnd. #gV\]U\]cb"U\]d"cf\[#VcbYbh#U\]d#ci fbU'#Jd`#-&#* 3j Yf1dXZVtj](#)

[Di V\]g\YX VmiH.Y'5-D' Di V\]g\\]b\[](#)

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[-bYf!VUbX'cdhcY'YVfcb\]WdfcdYfj\]Yg:\]b'ei Ubh a 'Xchgfri Vh fy'cZ'ck 'VUbX'\[Ud'==J 'gYa \]VcbXi Vtcfj'](#)



Calculated natural band offsets of all II–VI and III–V semiconductors: Chemical trends and the role of cation d orbitals

Su-Huai Wei^{a)} and Alex Zunger^{b)}

National Renewable Energy Laboratory, Golden, Colorado 80401

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Using first-principles all-electron band structure method, we have systematically calculated the natural band offsets DE_v between all II–VI and separately between III–V semiconductor compounds. Fundamental regularities are uncovered: for common-cation systems DE_v decreases when the cation atomic number increases, while for common-anion systems DE_v decreases when the anion atomic number increases. We find that coupling between anion p and cation d states plays a decisive role in determining the absolute position of the valence band maximum and thus the observed chemical trends. © 1998 American Institute of Physics. ©S0003-6951-98!03316-6#

The offset $DE_v(AX/BY)$ between the valence $\sim v!$ band maxima of two semiconductor compounds AX and BY forming a heterostructure is one of the most important parameters in interfacial structures deciding both transport and quantum confinement. Extensive studies ~see review in Ref. 1! have been carried out in the past to both measure and calculate DE_v of II–VI and III–V semiconductor compounds. However, most of the experimental studies concerned only a particular pair and their results are somewhat scattered. Furthermore, many of the previous theoretical calculations involved approximations ~e.g., model solid,² no p – d coupling,³ etc.! whose validity has not been verified. Thus, overall regularities and trends were not apparent. In this letter we have systematically calculated the natural band offsets DE_v via *ab initio*, all-electron band structure method⁴ between all II–VI

~i! Most valence band offsets are nonzero. This is in contrast with the “common-anion rule”^{12,13,3} that suggested that the offset between two semiconductors having the same anion will be small. The smallest DE_v occur between Zn/Cd and Ga/In common-anion systems ~Table I!

~

ergy and higher cation d orbital energy!. Figure 2 shows schematically how the $p-d$ coupling affects the band offset:

~a! Trend ~