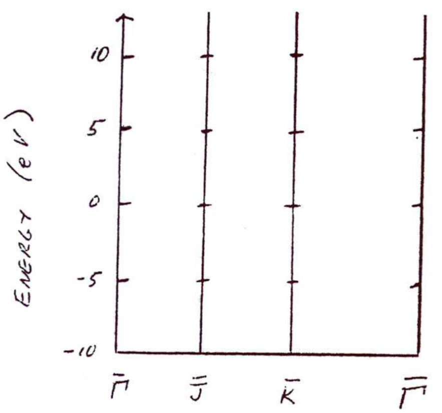
2) Consider the (001) surface of an insulating simple-cubic substrate having bulk lattice constant a. (Thus, the surface normal is **z**, and the surface unit cell is just an $a \times a$ square.) Assume that the lowest conduction band of the insulating substrate has bulk dispersion,

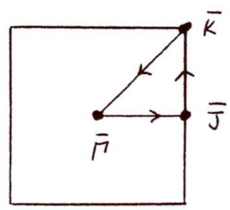
$$\varepsilon(k_x, k_y, k_z) = E_0 + 2V[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)]$$

where E_o=3.2eV and V = 1.1eV. Also, assume that higher bulk conduction (unoccupied) bands are sufficient high in energy, and all bulk valence (occupied) bands are sufficiently low in energy, to be of the problem.

a) Plot the projected bulk band structure of this unoccupied band along the line segments

$\bar{\Gamma} - \bar{J}, \bar{J} - \bar{K}$, and $\bar{K}$-$\bar{\Gamma}$ in the surface Brillouin zone. (Construct your plot in three adjacent panels in the conventional way illustrated in the figure below. The labeling in the surface Brillouin zone is shown; thus $\bar{\Gamma} - \bar{J}$ s means $(k_x, k_y)=(t, 0)$ for t going from 0 to π/a, etc.





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b) Now, chemisorbed on the surface is one Na atom per surface cell. We will make the approximation of treating this metallic surface layer as a free electron gas confined to a region of thickness d near the surface. That is, we take $\bar{\Gamma} - \bar{J}, \bar{J} - \bar{K}$, and $\bar{K}$-$\bar{\Gamma}$ (x, y, z) = V_0; for 0<z<d, and +∞ otherwise (the substrate is at z < 0). Calculate E (k_x, k_y) for the lowest energy band (corresponding to the ground state sinusoidal solution in the z-direction.), taking a = 3.0Å, d =3.5 Å, and V_o = - 8.9 eV (Note that $\hbar^2/2m$ = 3.81 Å). Add this band to your plot, indicating it as solid line where it is a surface state.