Band-gap engineering by III-V infill in sodalite.

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We study the structure of III-V clusters in sodalite by *ab initio* Molecular Dynamics (Car-Parrinello) and find strong bonding of the group III atoms to the oxygens of the cage with loss of tetrahedral order. The clusters introduce optically active states in the zeolite energy gap and turn it into a semiconductor with energy gap determined by its chemical nature rather than by quantum confinement. Within the Local Density Approximation we find values of $\approx$ 0.4 eV and $\approx$ 1.9 eV for InAs and GaN clusters of the same size. We suggest that the growth of selected compounds in zeolite may lead to wide gap semiconductors for blue light emitting devices.