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**Density functional study of the effects of doping and stoichiometry on gallium diffusion in gallium arsenide** J.T. SCHICK, Villanova Univ., C.G. MORGAN, Wayne State Univ. — Previous experimental [1-4] and theoretical [5,6] work on the properties of diffusion of gallium within gallium arsenide has produced some results that are apparently at odds with each other. We present results of a wide theoretical survey of the point defects that form in this material with special attention paid to the formation and diffusion of excess-gallium-related point defects. In this study we applied density functional theory in the local density approximation [7]. Diffusion was examined through the use of the nudged elastic band method [8]. After considering the accuracy of the approximations used, the calculations yield information compatible with the experimental situation and capable of shedding light on areas of apparent disagreement.

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