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First-principles lineshapes of defect luminescence bands AUDRIUS ALKAUSKAS, DANIEL STEIAUF, JOHN L. LYONS, CHRIS G. VAN DE WALLE, University of California Santa Barbara — We present a theoretical study of broadening of defect luminescence bands due to vibronic coupling. Numerical proof is provided for the commonly used assumption that a multi-dimensional vibrational problem can be mapped onto an effective one-dimensional configuration coordinate diagram. Our approach is implemented based on density functional theory with a hybrid functional, resulting in luminescence lineshapes for important defects in GaN and ZnO that show unprecedented agreement with experiment. We find clear trends concerning effective parameters that characterize luminescence bands of donor- and acceptor-type defects, thus facilitating their identification.

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