

Abstract Submitted
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The chemical trends of a new defect cluster: DDX centers JIE MA, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — DX center is a major “killer” defect limiting n-type doping in group II-VI and III-V semiconductors. It converts a shallow donor to deep one, which is a major reason for the saturation of free-electron carriers in the doping process. Several structure models of isolated DX centers have been proposed in the literatures, such as the broken-bond model (BB-DX), and the α and β cation-cation bond model (CCB-DX). All these DX centers can be stabilized with hydrostatic pressure or reduced dimensionality and size. In group III-V and II-VI semiconductors, it has been common believe that cation-site induced DX centers are easier to form than anion-site induced ones. Because DX centers trap an extra electron, therefore, another defect in the system must donate the electron and form a positive charged defect. We show, using GaAs as an example, that in heavily doped semiconductor, the negative charged DX center and positive charged donor can couple strongly through the Coulomb interaction, forming the dominant DDX center. The DDX centers are still deep level defects. However, unlike the DX center, the DDX centers have different chemical trends, i.e., anion-site DDX center is easier to form than cation-site DDX centers. A simple model is proposed to explain the new trends.

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