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The first excitonic absorption peak in the cubic KMgF₃ crystal derived from Bethe-Salpeter equation

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We obtained the values of the indirect $\Gamma - R$ band gaps as follows: 6.99 eV from the GGA and 11.72 eV from the GW approaches, respectively. The fundamental band gap found from optical absorption is 10.8 eV. The last two values differ from each other by 0.92 eV. The reason for this difference, we will seek on base of the results, obtained from the Bethe-Salpeter equation [1].
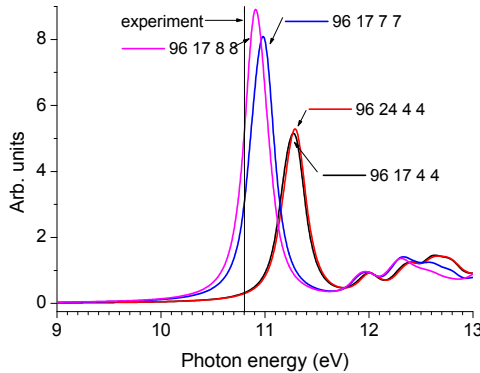

Fig 1. The dielectric constant $\varepsilon_2(E)$ evaluated from Bethe-Salpeter equation.

As can be seen from Fig.1, the curve obtained involving in calculation 96 bands, the maximum energy 34 Ry (17 Ha), 8 valence and 8 conduction band states, included into transition subspace, shows good agreement with experiment. All the calculations have been done by means of ABINIT code [1].

1. *Gonze X., Jollet F., Abreu Araujo F., Adams D., Amadon B.et al.* Recent developments in the ABINIT software package // Computer Phys. Comm.- 2016.-**205.-**P. 106-131.