branching plane

At a *conical intersection* point, the plane spanned by the gradient difference vector ($\boldsymbol{x}_1$) and the gradient of the interstate coupling vector ($\boldsymbol{x}_2$):

$$\boldsymbol{x}_1 = \frac{\partial(E_2 - E_1)}{\partial Q}\boldsymbol{q}$$

$$\boldsymbol{x}_2 = \left\langle \boldsymbol{C}_1^t \left(\frac{\partial H}{\partial Q}\right) \boldsymbol{C}_2 \right\rangle \boldsymbol{q}$$

where $\boldsymbol{C}_1$ and $\boldsymbol{C}_2$ are the configuration interaction eigenvectors (i.e., the excited and ground-state *adiabatic* wavefunctions) in a conical intersection problem, H is the conical intersection Hamiltonian, $\boldsymbol{Q}$ represents the nuclear configuration vector of the system, and thus $\boldsymbol{q}$ is a unit vector in the direction of vector $\boldsymbol{Q}$. E_1 and E_2 are the energies of the lower and upper states, respectively.
Note: The branching plane is also referred to as the ***g-h*** plane. Inspection of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ provides information on the geometrical deformation imposed on an *excited state* molecular entity immediately after decay at a conical intersection. Consequently, these vectors provide information on the *ground-state* species that will be formed after the decay.

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