David R. Yarkony Department of Chemistry , Johns Hopkins University June 2022 MQM Abstract

Diabatics

The talk is divided into 3 parts discussing

- (i) the defining conditions of a diabatic basis and the consequences,
- (ii) the likelihood that properties based, legacy, diabatization will fail if used to construct a global diabatization
- (iii) use in constructing diabatic potential energy matricies (DPEM) which incorporate the spin-orbit interaction within the spin diabatic basis approximation

r