**PEPTIDE HYDROLYSIS CATALYZED BY A B-CYCLODEXTRIN CONJUGATED PD(II) COMPLEX**. Xiaoxia Zhu, Rajeev Prabhakar, Department of chemistry, University of Miami, 1301 Memorial Drive, Coral Gables, FL 33146.

The mechanism for the hydrolysis of the X-Pro peptide bond in the X-Pro-Phe sequency (X→ amino acid) by a β-cyclodextrin (β-CD) conjugated Pd(II) complex (**$I_{MPC}$-βCD**) has been investigated using QM(B3LYP) and QM/MM(B3LYP/Amber) approaches. The **$I_{MPC}$-βCD** complex utilizes β-CD to selectively bind to the substrate and the Pd(II) center to catalyze the hydrolysis of the peptide bond. Based on experimental information, two kinetically indistinguishable mechanisms have been proposed: (1) external water attack mechanism and (2) internal water delivery mechanism. Our DFT calculations show that among these two mechanisms, the internal water mechanism is energetically feasible and occurs with 14.3 kcal/mol lower barrier than the external water delivery mechanism. This mechanism was subsequently utilized to explore the optimal number and the binding modes of β-CD using the QM/MM approach.