

FMB_n (FM=Fe, Co, Ni; $n=1-12$)团簇结构和电子性质

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Cluster Structures and Electronic Properties of FMB_n

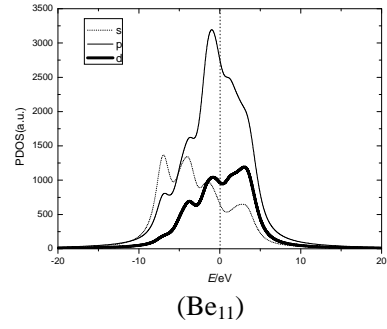
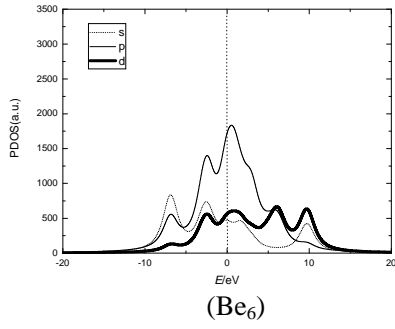
(FM=Fe, Co, Ni; $n=1-12$) Clusters

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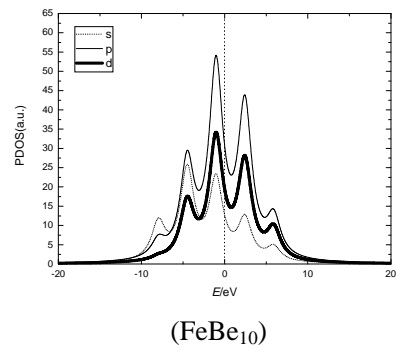
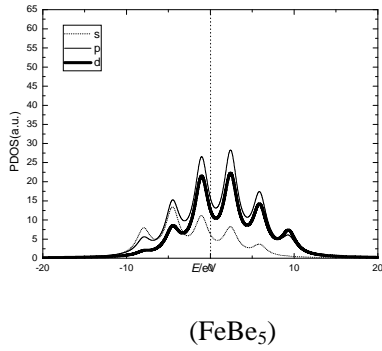
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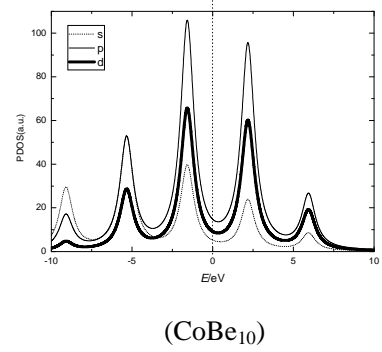
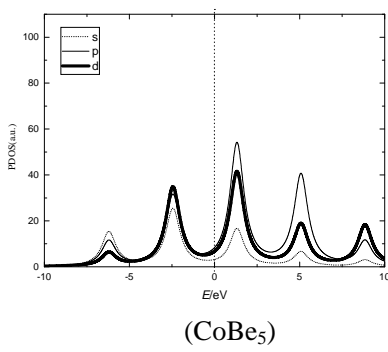
Be_{n+1} ($n=5, 10$)



FeBe_n ($n=5, 10$)



CoBe_n ($n=5, 10$)



NiBe_n ($n=5, 10$)

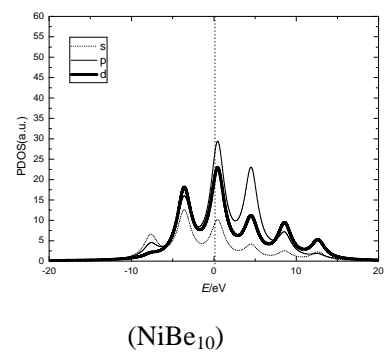
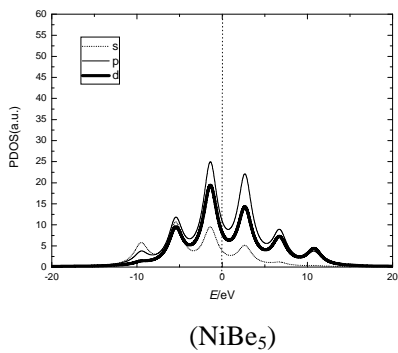


图 S1 FMBe_n ($n=5, 10$)和 Be_{n+1} ($n=5, 10$)团簇 s 、 p 、 d 轨道的 PDOS

Fig.S1 Partial density of states (PDOS) of s , p , d orbits for FMBe_n ($n=5, 10$) and Be_{n+1} ($n=5, 10$) clusters