

Transition metalides based on facially polarized *all-cis*-1,2,3,4,5,6-hexafluorocyclohexane – a new class of high performance second order nonlinear optical materials

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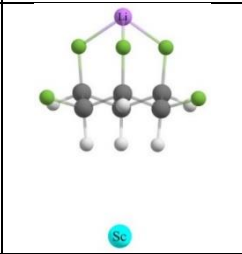
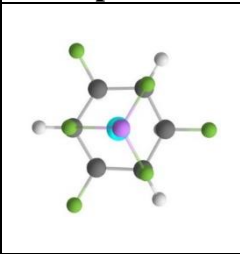
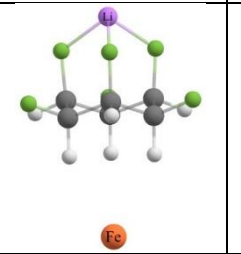
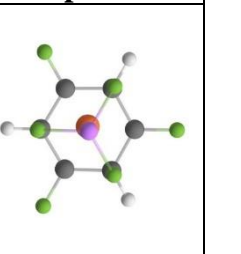
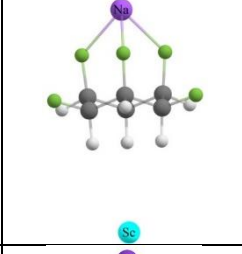
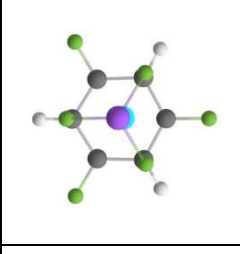
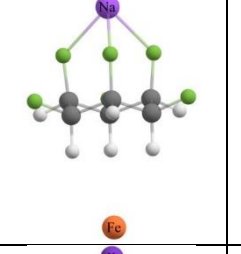
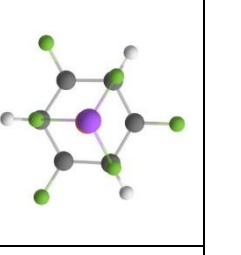
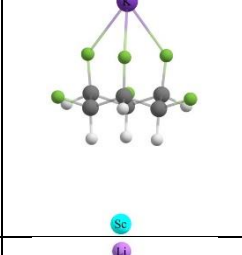
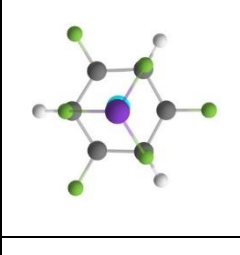
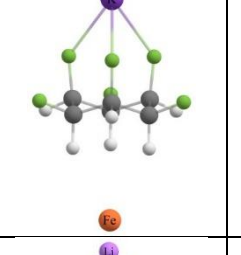
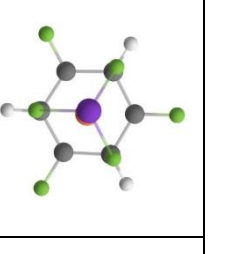
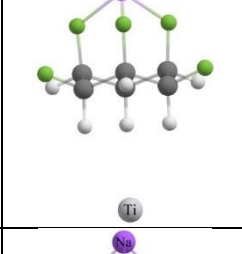
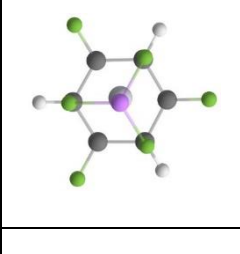
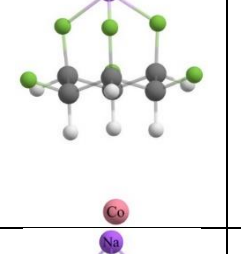
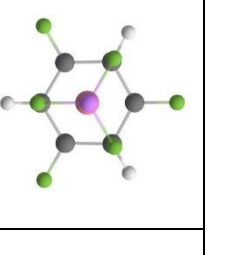
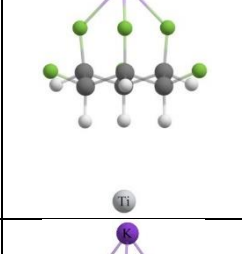
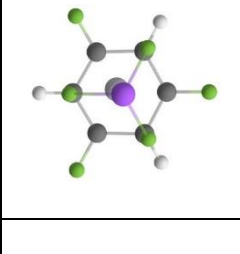
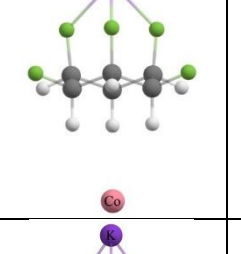
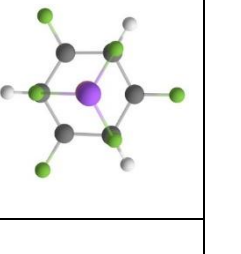
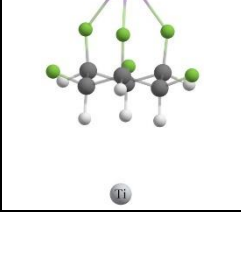
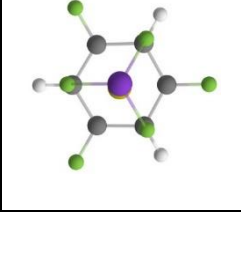
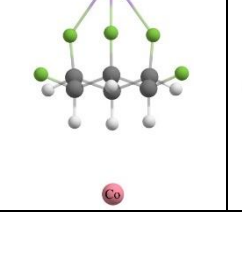
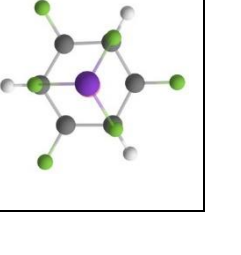
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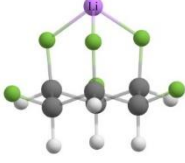
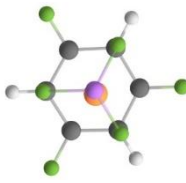
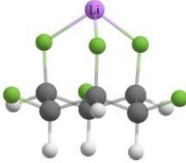
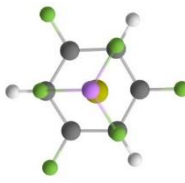
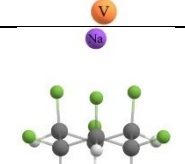

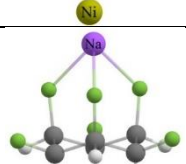
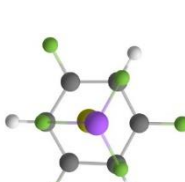
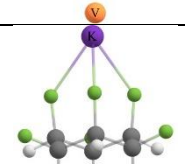

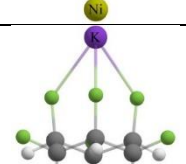

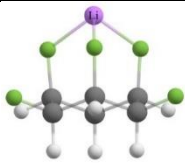

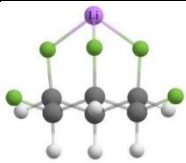

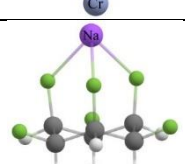
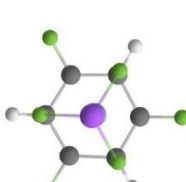
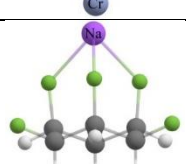

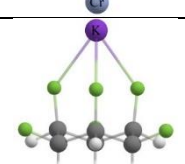

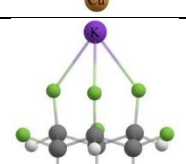
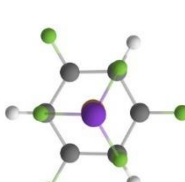
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Complex	Side view	Top View	Complex	Side view	Top View
Li-J-Sc			Li-J-Fe		
Na-J-Sc			Na-J-Fe		
K-J-Sc			K-J-Fe		
Li-J-Ti			Li-J-Co		
Na-J-Ti			Na-J-Co		
K-J-Ti			K-J-Co		

Li-J-V			Li-J-Ni		
Na-J-V			Na-J-Ni		
K-J-V			K-J-Ni		
Li-J-Cr			Li-J-Cu		
Na-J-Cr			Na-J-Cu		
K-J-Cr			K-J-Cu		

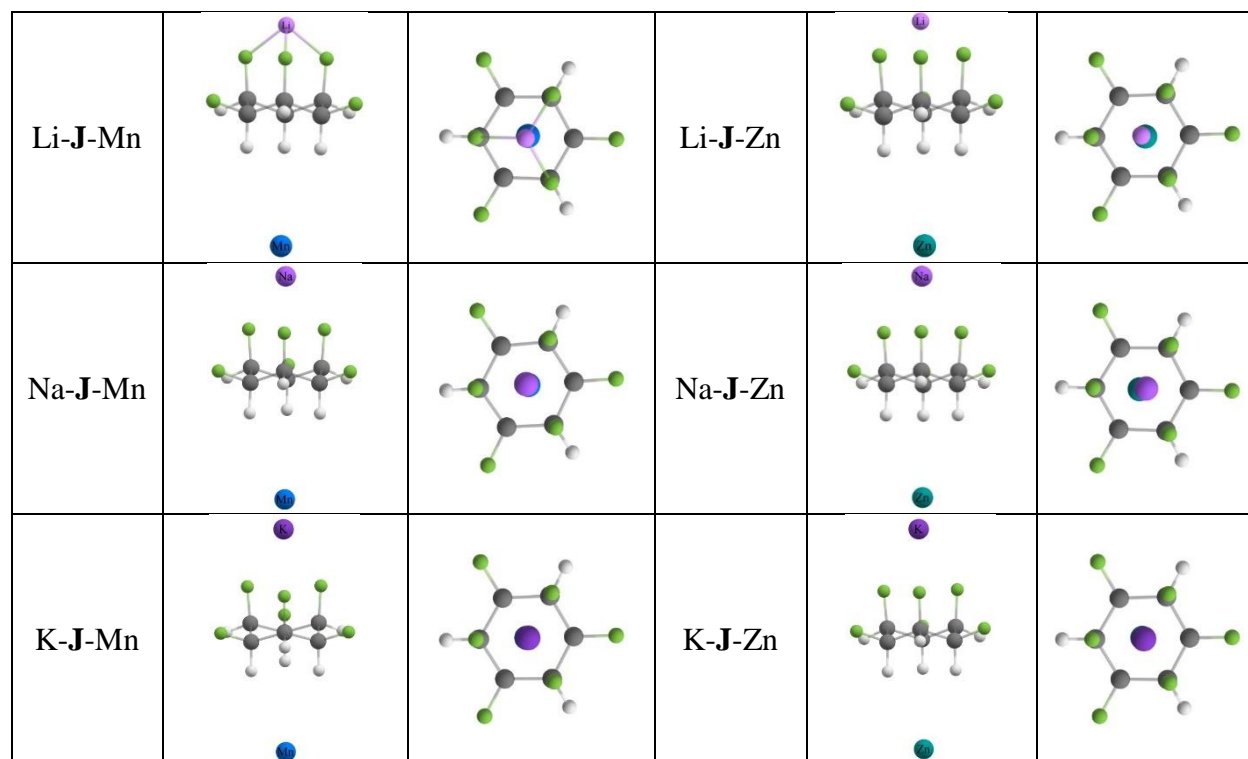
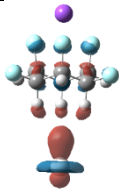
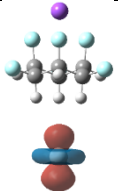
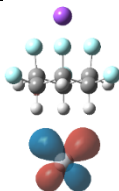
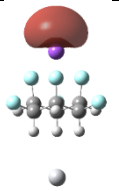
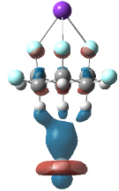
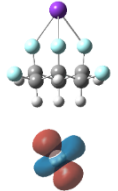
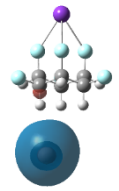
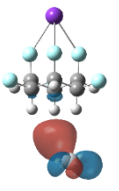
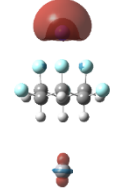
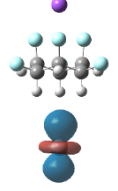
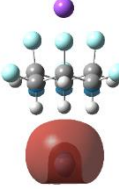
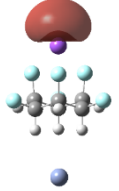
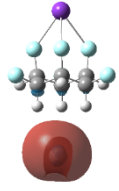
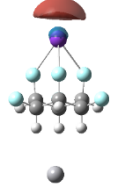
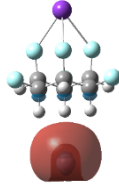
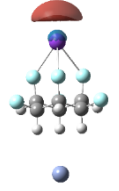
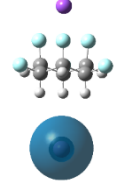
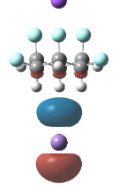
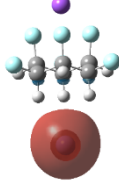

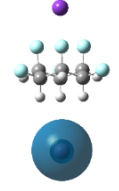
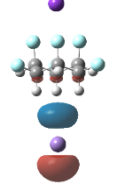
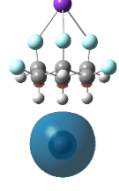
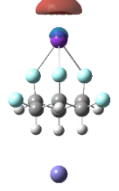


Figure S1 Optimized structures of transition metalides $\text{TM}^-1\text{-AM}^+$ ($\text{TM}^- = \text{Sc-Zn}$; $\text{AM}^+ = \text{Li, Na, K}$)

HOMO	LUMO	HOMO	LUMO
			
Na-J-Sc		Na-J-Ti	
			
K-J-Sc		K-J-Ti	
			
Na-J-V		Na-J-Cr	
			
K-J-V		K-J-Cr	
			
Na-J-Mn		Na-J-Fe	
			
K-J-Mn		K-J-Fe	

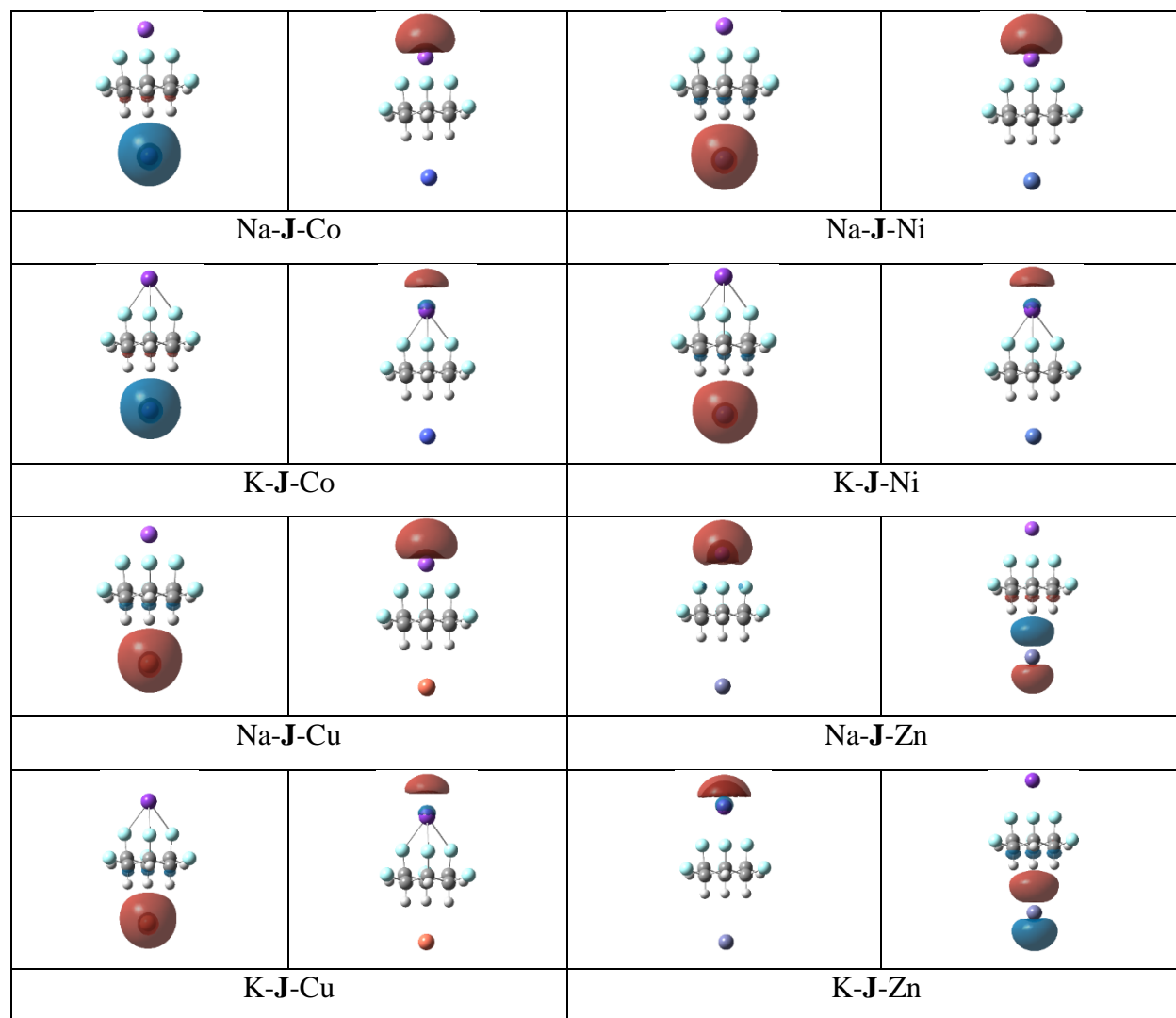


Figure S2 HOMO-LUMO densities of TM^- -1- AM^+ ($\text{TM}^- = \text{Ti, Cr, Fe, Ni, and Zn}$; $\text{AM}^+ = \text{Na, K}$)