Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Magnetism and perfect spin filtering in pristine $MgCl_2$ nanoribbons modulated by edge modification

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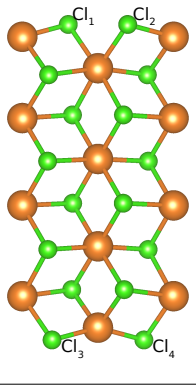
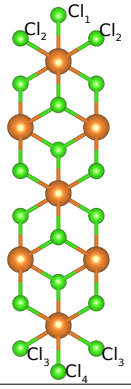
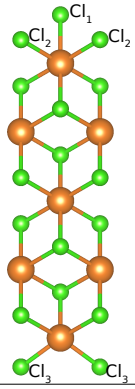
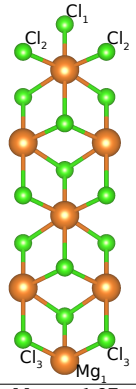
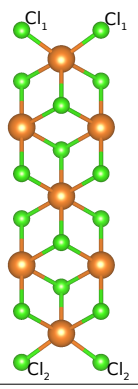
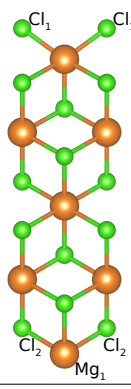
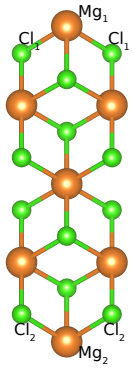
Table S1 Bader charge analysis of all the studied N = 4 $AMgCl_2$ and $ZMgCl_2$ nanoribbons. Orange and green spheres represent Mg and Cl atoms, respectively.

	Armchair	$Cl_\alpha Cl_\alpha$	$Cl_\alpha Cl_\beta$	$Cl_\alpha Mg$	$Cl_\beta Cl_\beta$	$Cl_\beta Mg$	MgMg
							
Net effective charge	Mg ≈ +1.97 Cl ≈ -1.0 Cl_{1-4} ≈ -0.97	Mg ≈ +1.97 Cl ≈ -1.0 $Cl_{1,4}$ ≈ -0.36 $Cl_{2,3}$ ≈ -0.63	Mg ≈ +1.98 Cl ≈ -1.0 Cl_1 ≈ -0.36 Cl_2 ≈ -0.63 Cl_3 ≈ -0.97	Mg ≈ +1.97 Cl ≈ -1.0 Mg_1 ≈ +1.58 Cl_1 ≈ -0.45 Cl_2 ≈ -0.82 Cl_3 ≈ -1.21	Mg ≈ +1.98 Cl ≈ -1.0 $Cl_{1,2}$ ≈ -0.98	Mg ≈ +1.98 Cl ≈ -1.0 Mg_1 ≈ +1.23 Cl_1 ≈ -1.16 Cl_2 ≈ -0.97	Mg ≈ +1.98 Cl ≈ -1.0 $Mg_{1,2}$ ≈ +1.22 $Cl_{1,2}$ ≈ -1.16