



Theoretical Prediction on Half-Metallic Antiferromagnets in Strongly Correlated Systems



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Classification of materials

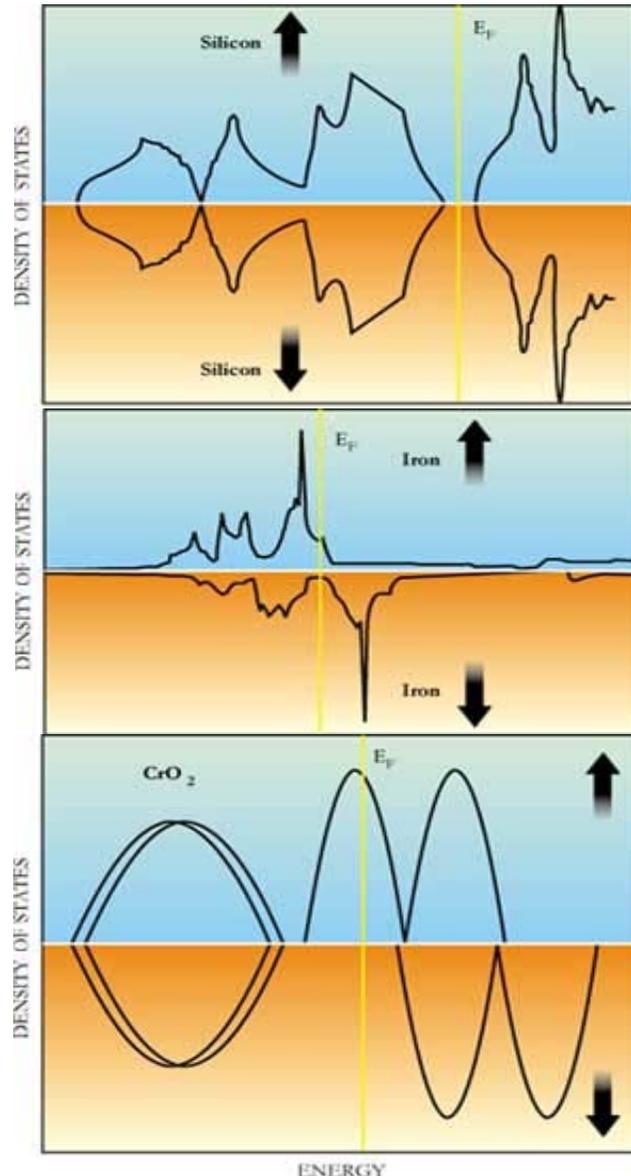
□ Density of states

□ Half metal

○ spin-up e metallic

○ spin-down e insulating

usually magnetic,
integer μ_B per unit cell



semiconductor

ferromagnet

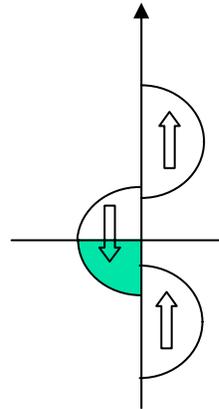
half metal

*Pickett and Moodera,
Physics Today (2001)*

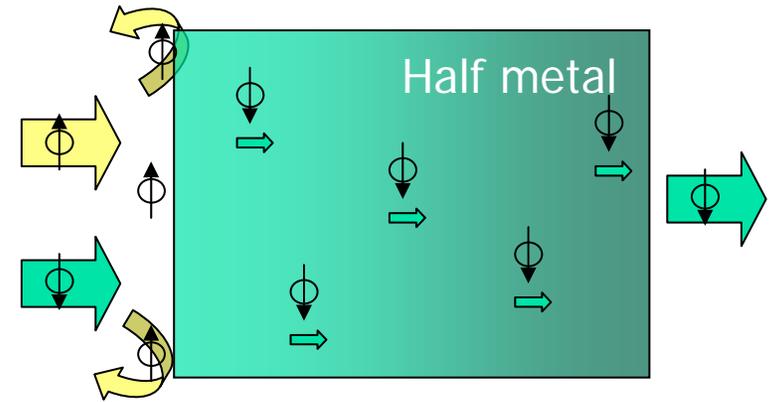
Ideal material for spintronics

□ Half metal

de Groot et al.
(1983)

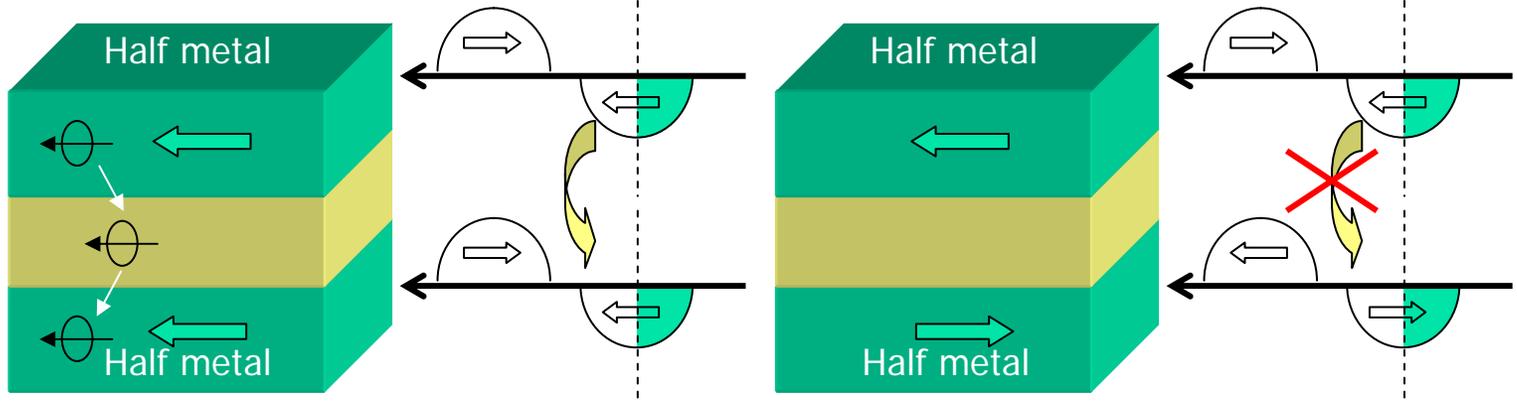


○ emitter for spin-polarized e's



□ Infinite MR:

MR = 1800% $\text{La}_2\text{SrMn}_3\text{O}_9$ at low temperature

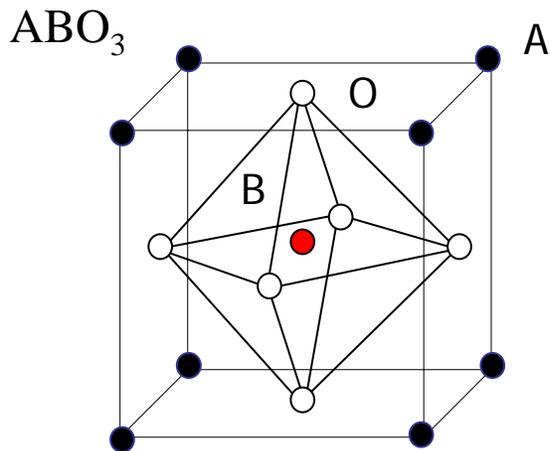


□ Known HM: CrO_2 ($T_c=340\text{K}$), NiMnSb ($T_c=728\text{K}$), $\text{Sr}_2\text{FeMoO}_6$ ($T_c=635\text{K}$)

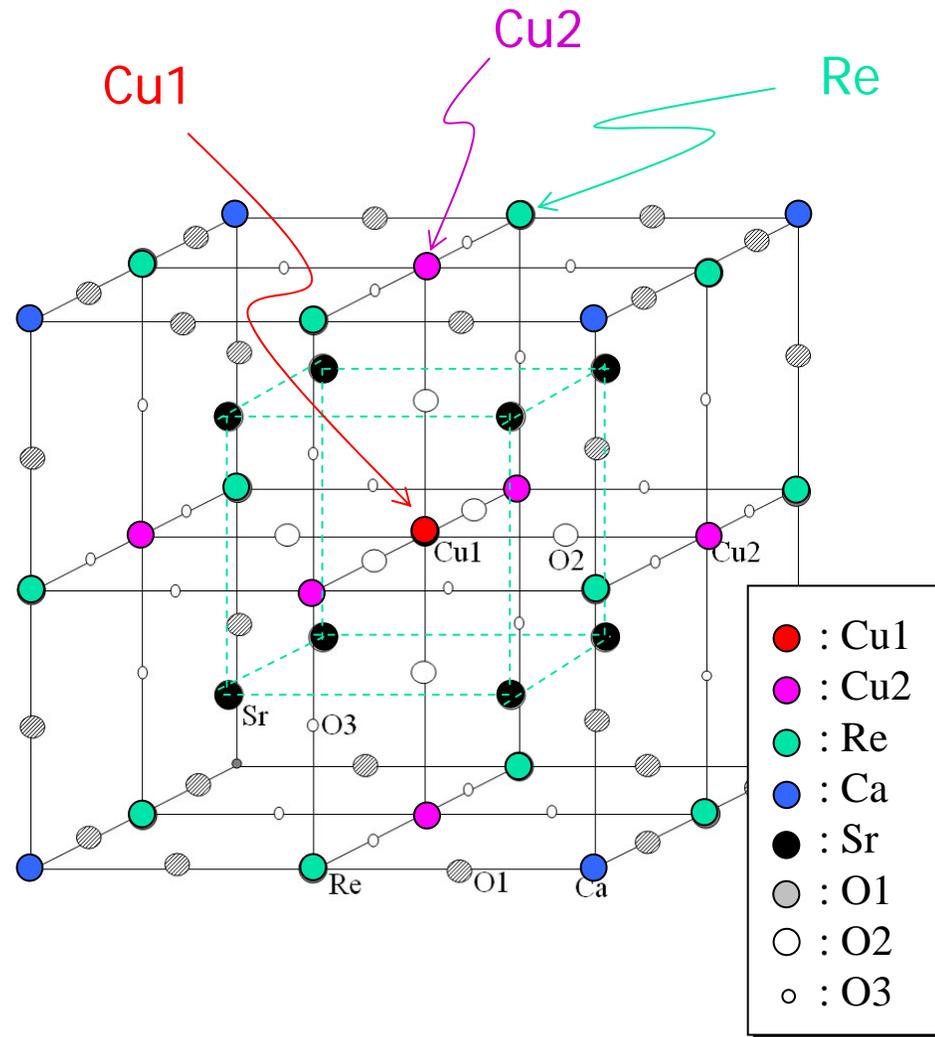
New cuprate $\text{Sr}_8\text{CaRe}_3\text{Cu}_4\text{O}_{24}$

Takayama-Muromati et al. (2003)

- Ferrimagnetic insulator: $T_c = 440\text{K}$, $\mu_{\text{tot}} = 1\mu_B$ @ $T = 0$
- Structure: perovskite



- ◇ A site: Sr atoms
- ◇ B site: Ca, Re and Cu atoms in an ordered way
- ◇ Oxygen octahedron

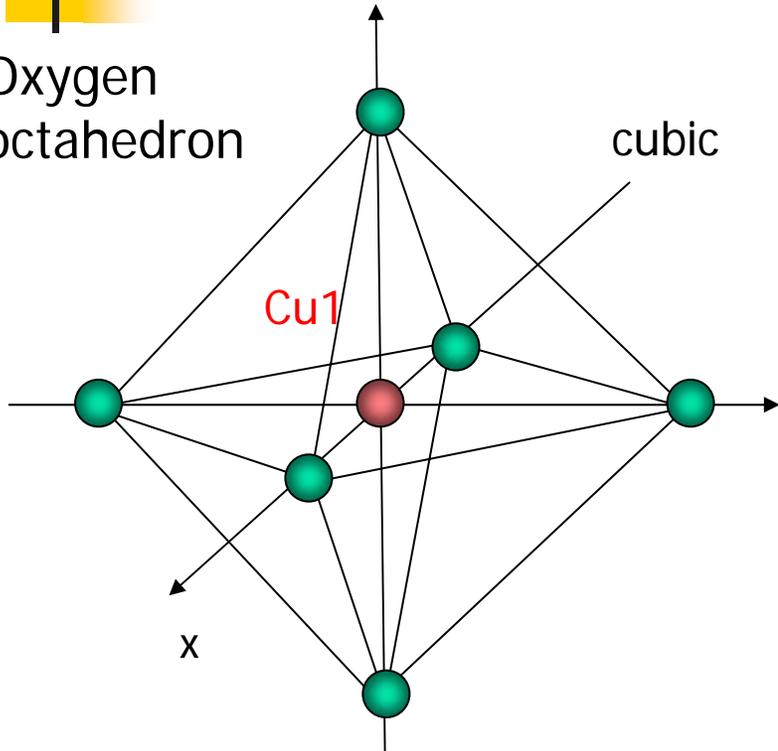


d orbitals and oxygen octahedron

Oxygen octahedron

cubic

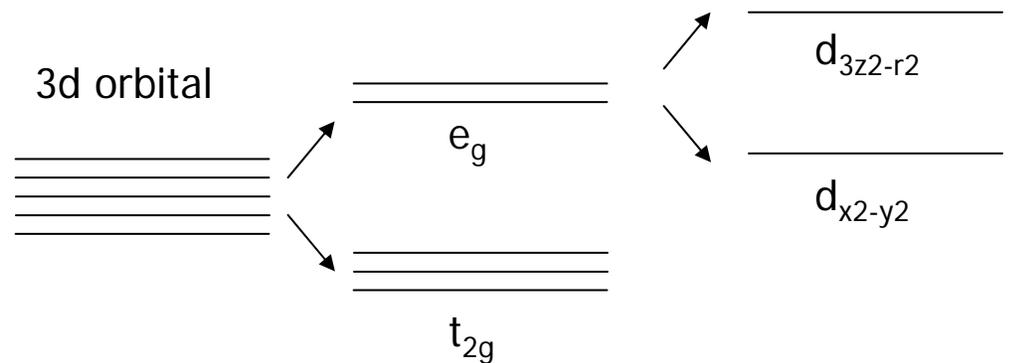
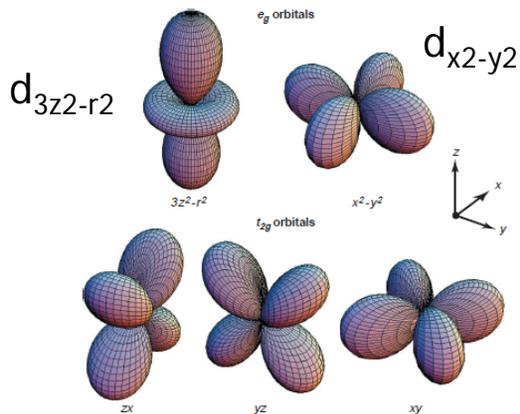
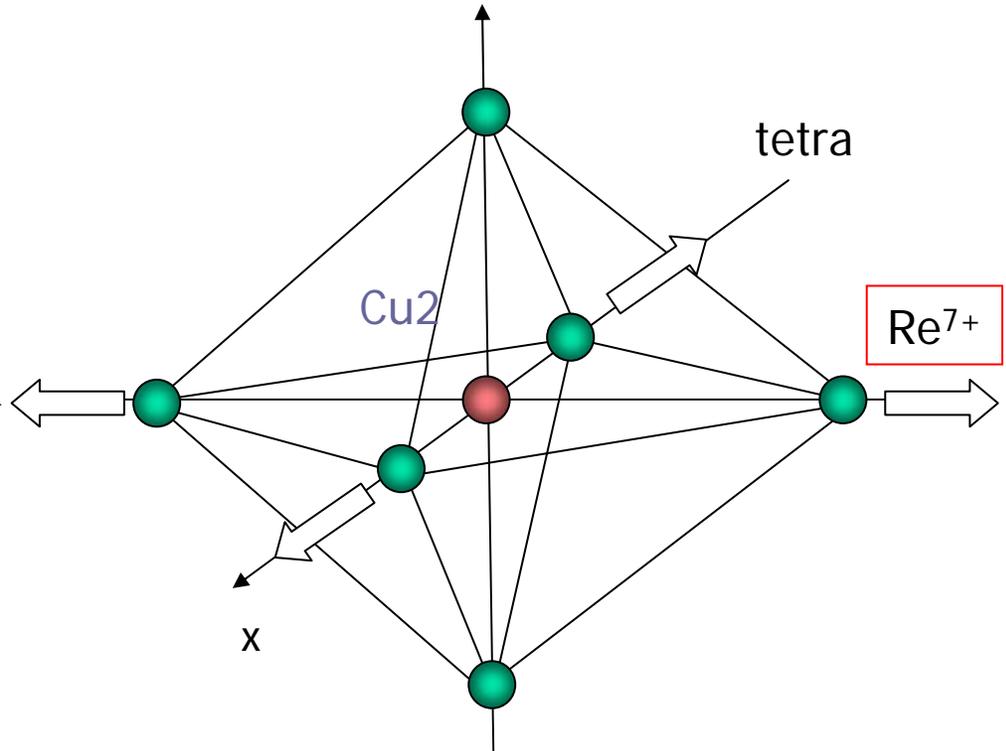
Cu¹⁺



tetra

Cu²⁺

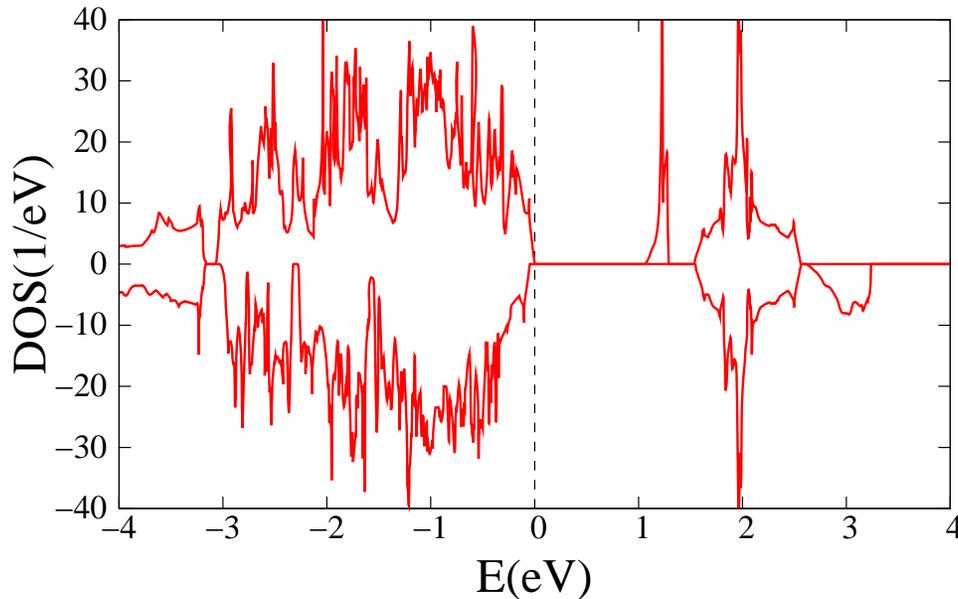
Re⁷⁺



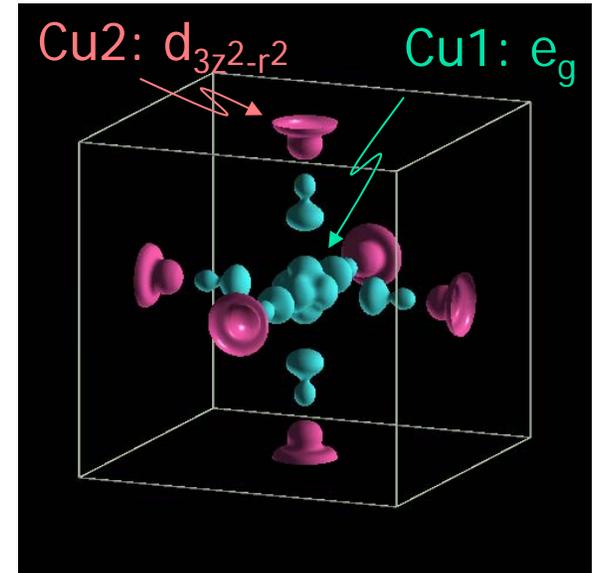
$\text{Sr}_8\text{CaRe}_3\text{Cu}_4\text{O}_{24}$

Wan, Kohno and Hu: PRL (2005)
 Nie and Hu: PRL (2008)

- DOS: DFA+U
 VASP package ($U=10\text{eV}$, $J=1.2\text{eV}$)



- Spin-magnetization distribution



- charge, orbital and spin orders

- total magnetization
 ferrimagnetic state of

Cu1: Cu^{3+} : $3d^8$ e_g $S=1$ X 1

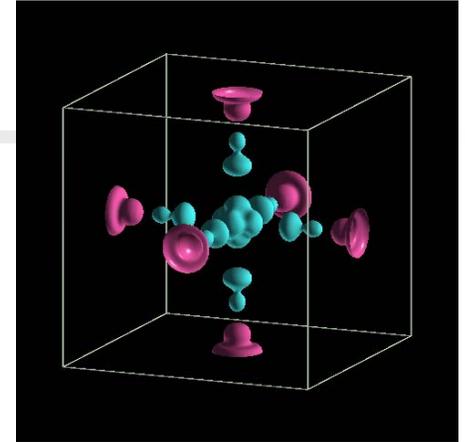
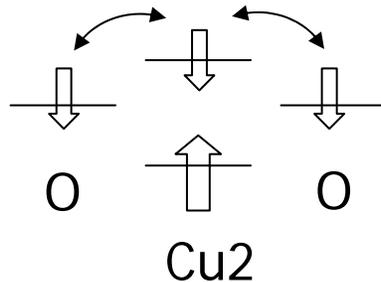
$\mu_{\text{tot}} = 1\mu_B$ per unit cell

Cu2: Cu^{2+} : $3d^9$ $d_{3z^2-r^2}$ $s=1/2$ X 3

○ agree with experiments

Spin of Oxygen

- charge-transfer effect



→ O-2p band with **down spin** presumes **lower energy** (anti-parallel to Cu²⁺ majority spin)

- Anderson model: antiferromagnetic scattering of conduction electrons by a single magnetic impurity

- Idea for charge-spin-orbital manipulation

hole should go to O-2p band with **up spin**

- cancel total spin $+1\mu_B$
- generate finite DOS at FL

Periodic Table

PERIODIC TABLE										NIST		18														
Atomic Properties of the Elements										National Institute of Standards and Technology		VIII A														
										Technology Administration, U.S. Department of Commerce																
										Physics Laboratory		Standard Reference Data Group														
										physics.nist.gov		www.nist.gov/srd														
										13		14		15		16		17		18						
										IIIA		IVA		VA		VIA		VIIA		VIII A						
1 1s 13.5984	2 IIA		Frequently used fundamental physical constants For the most accurate values of these and other constants, visit physics.nist.gov/constants 1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³ Cs speed of light in vacuum <i>c</i> 299 792 458 m s ⁻¹ (exact) Planck constant <i>h</i> 6.6261 × 10 ⁻³⁴ J s (<i>h</i> = <i>h</i> 2π) elementary charge <i>e</i> 1.6022 × 10 ⁻¹⁹ C electron mass <i>m_e</i> 9.1094 × 10 ⁻³¹ kg <i>m_ec²</i> 0.5110 MeV proton mass <i>m_p</i> 1.6726 × 10 ⁻²⁷ kg fine-structure constant <i>α</i> 1/137.036 Rydberg constant <i>R_∞</i> 10 973 732 m ⁻¹ <i>R_∞c</i> 3.289 842 × 10 ¹⁵ Hz <i>R_∞hc</i> 13.6057 eV <i>R_∞hc</i> 1.3807 × 10 ⁻²³ J K ⁻¹ Boltzmann constant <i>k</i>										5 1s ² 2s ² 2p ¹	6 1s ² 2s ² 2p ²	7 1s ² 2s ² 2p ³	8 1s ² 2s ² 2p ⁴	9 1s ² 2s ² 2p ⁵	10 1s ² 2s ² 2p ⁶	11 1s ² 2s ² 2p ⁶ 3s ¹	12 1s ² 2s ² 2p ⁶ 3s ²	13 1s ² 2s ² 2p ⁶ 3s ² 3p ¹	14 1s ² 2s ² 2p ⁶ 3s ² 3p ²	15 1s ² 2s ² 2p ⁶ 3s ² 3p ³	16 1s ² 2s ² 2p ⁶ 3s ² 3p ⁴	17 1s ² 2s ² 2p ⁶ 3s ² 3p ⁵	18 1s ² 2s ² 2p ⁶ 3s ² 3p ⁶
1 Hydrogen 1.00794	2 Helium 4.002602 1s ² 24.5674	3 Lithium 6.941 1s ² 2s ¹ 5.3917	4 Beryllium 9.012182 1s ² 2s ² 9.3227	5 Boron 10.811 1s ² 2s ² 2p ¹ 8.2980	6 Carbon 12.0107 1s ² 2s ² 2p ² 11.2603	7 Nitrogen 14.0067 1s ² 2s ² 2p ³ 14.5341	8 Oxygen 15.9994 1s ² 2s ² 2p ⁴ 13.6181	9 Fluorine 18.9984032 1s ² 2s ² 2p ⁵ 17.4228	10 Neon 20.1797 1s ² 2s ² 2p ⁶ 21.5645	11 Sodium 22.989770 [Ne]3s ¹ 5.1391	12 Magnesium 24.3050 [Ne]3s ² 7.6462	13 Aluminum 26.981538 [Ne]3s ² 3p ¹ 5.9858	14 Silicon 28.0855 [Ne]3s ² 3p ² 8.1517	15 Phosphorus 30.973761 [Ne]3s ² 3p ³ 10.4857	16 Sulfur 32.065 [Ne]3s ² 3p ⁴ 10.3600	17 Chlorine 35.453 [Ne]3s ² 3p ⁵ 12.9676	18 Argon 39.948 [Ne]3s ² 3p ⁶ 15.7596									
19 Potassium 39.0983 [Ar]4s ¹ 4.3407	20 Calcium 40.078 [Ar]4s ² 6.4472	21 Scandium 44.955910 [Ar]3d ¹ 4s ² 6.5615	22 Titanium 47.867 [Ar]3d ² 4s ² 6.8281	23 Vanadium 50.9415 [Ar]3d ³ 4s ² 6.7462	24 Chromium 51.9961 [Ar]3d ⁵ 4s ¹ 6.7665	25 Manganese 54.938049 [Ar]3d ⁵ 4s ² 7.4340	26 Iron 55.845 [Ar]3d ⁶ 4s ² 7.9024	27 Cobalt 58.933200 [Ar]3d ⁷ 4s ² 7.8810	28 Nickel 58.6934 [Ar]3d ⁸ 4s ² 7.6398	29 Copper 63.546 [Ar]3d ¹⁰ 4s ¹ 9.3942	30 Zinc 65.409 [Ar]3d ¹⁰ 4s ² 9.2644	31 Gallium 69.723 [Ar]3d ¹⁰ 4s ² 4p ¹ 5.9993	32 Germanium 72.64 [Ar]3d ¹⁰ 4s ² 4p ² 7.8994	33 Arsenic 74.92160 [Ar]3d ¹⁰ 4s ² 4p ³ 9.7886	34 Selenium 78.95 [Ar]3d ¹⁰ 4s ² 4p ⁴ 9.7524	35 Bromine 79.904 [Ar]3d ¹⁰ 4s ² 4p ⁵ 11.8138	36 Krypton 83.796 [Ar]3d ¹⁰ 4s ² 4p ⁶ 13.9996									
37 Rubidium 85.4678 [Kr]5s ¹ 4.1771	38 Strontium 87.62 [Kr]5s ² 5.6949	39 Yttrium 88.90585 [Kr]4d ¹ 5s ² 5.2173	40 Zirconium 91.224 [Kr]4d ² 5s ² 6.6339	41 Niobium 92.90638 [Kr]4d ⁴ 5s ¹ 6.7589	42 Molybdenum 95.94 [Kr]4d ⁵ 5s ¹ 7.0924	43 Technetium (98) [Kr]4d ⁵ 5s ² 7.28	44 Ruthenium 101.07 [Kr]4d ⁷ 5s ¹ 7.3605	45 Rhodium 102.90550 [Kr]4d ⁸ 5s ¹ 7.4589	46 Palladium 106.42 [Kr]4d ¹⁰ 8.3369	47 Silver 107.8682 [Kr]4d ¹⁰ 5s ¹ 7.5762	48 Cadmium 112.411 [Kr]4d ¹⁰ 5s ² 8.9938	49 Indium 114.818 [Kr]4d ¹⁰ 5s ² 5p ¹ 5.7864	50 Tin 118.710 [Kr]4d ¹⁰ 5s ² 5p ² 7.3439	51 Antimony 121.760 [Kr]4d ¹⁰ 5s ² 5p ³ 8.6084	52 Tellurium 127.60 [Kr]4d ¹⁰ 5s ² 5p ⁴ 9.0096	53 Iodine 126.90447 [Kr]4d ¹⁰ 5s ² 5p ⁵ 10.4513	54 Xenon 131.293 [Kr]4d ¹⁰ 5s ² 5p ⁶ 12.1296									
55 Cesium 132.90545 [Xe]6s ¹ 3.8939	56 Barium 137.327 [Xe]6s ² 5.2117	57 Lanthanum 138.90547 [Xe]4f ¹ 5d ¹ 6s ² 6.8251	72 Hafnium 178.49 [Xe]4f ¹⁴ 5d ² 6s ² 6.8251	73 Tantalum 180.9479 [Xe]4f ¹⁴ 5d ³ 6s ² 7.5496	74 Tungsten 183.84 [Xe]4f ¹⁴ 5d ⁴ 6s ² 7.8640	75 Rhenium 186.207 [Xe]4f ¹⁴ 5d ⁵ 6s ² 7.8335	76 Osmium 190.23 [Xe]4f ¹⁴ 5d ⁶ 6s ² 8.4382	77 Iridium 192.217 [Xe]4f ¹⁴ 5d ⁷ 6s ² 8.9670	78 Platinum 195.078 [Xe]4f ¹⁴ 5d ⁹ 6s ¹ 8.9588	79 Gold 196.96655 [Xe]4f ¹⁴ 5d ¹⁰ 6s ¹ 9.2255	80 Mercury 200.59 [Xe]4f ¹⁴ 5d ¹⁰ 6s ² 10.4375	81 Thallium 204.3833 [Hg]6p ¹ 6.1062	82 Lead 207.2 [Hg]6p ² 7.4167	83 Bismuth 208.98038 [Hg]6p ³ 7.2855	84 Polonium (209) [Hg]6p ⁴ 8.414	85 Astatine (210) [Hg]6p ⁵	86 Radon (222) [Hg]6p ⁶ 10.7485									

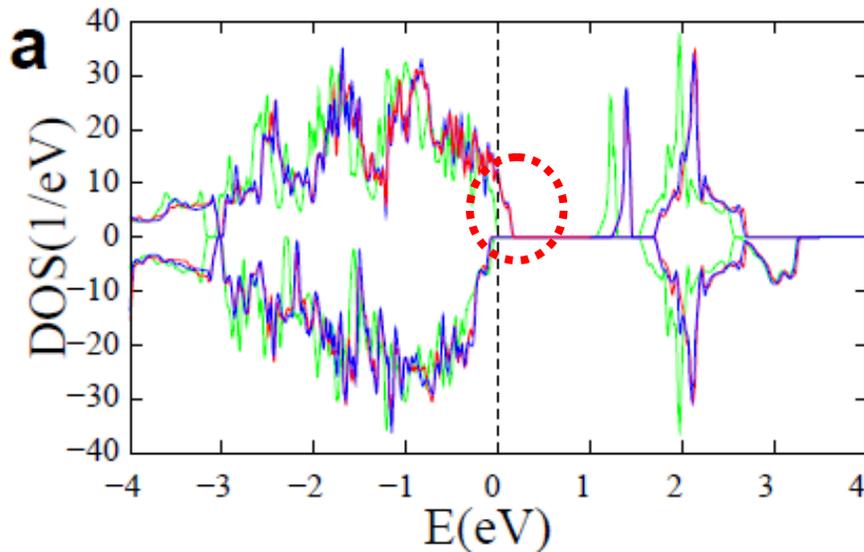


Sr₇RbCaRe₃Cu₄O₂₄

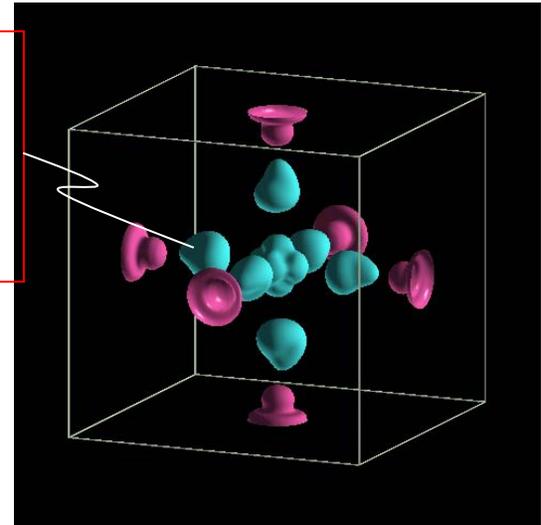
Nie and Hu: PRL (2008)

□ DOS: half-metallic

□ Spin-magnetization distribution



the hole goes to O, with fully up spin !

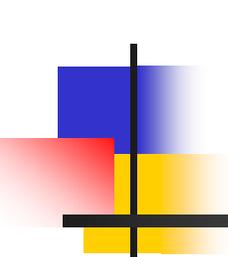


Half metallic antiferromagnet

□ spin-magnetic moments

van Leuken and de Groot (1995)

	$\mu_{\text{tot}} [\mu_B]$	Cu1	Cu2	O21	O22
undoped	1.0	-1.09	0.81	-0.07	
one hole	0.0	-1.08	0.82	-0.24	-0.13

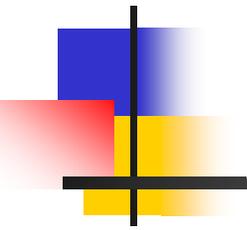


Summary

- Half metal: metallic in (only) one spin channel
 - most ideal material for spintronics, under intensive study

- Half metallic antiferromagnet **HMAFM**
 - spin-polarized current with magnetization totally compensate
 - not an oxymoron, not a scientific fiction

- Our proposal: strongly correlated electron systems
 - ferrimagnetic insulator with integer total magnetic moment
 - doping mobile carrier: substitution on A, B, and O sites
 - spin of doped carrier fully polarized due to strong coupling



Thank You!