

Supplementary Information

Optical response, lithiation and charge transfer in Sn-based 211 MAX phases with electron localization function

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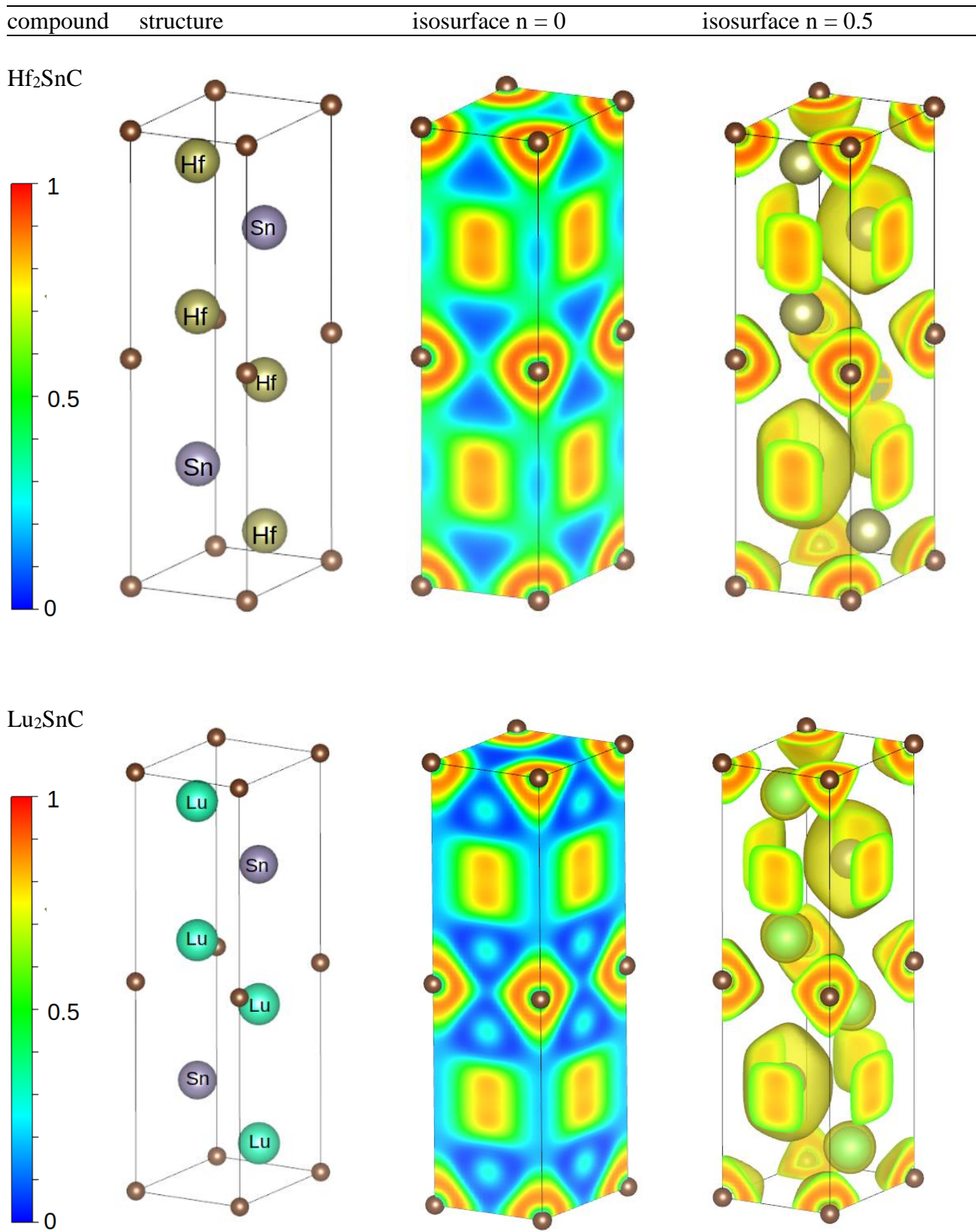
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Table S1. Optical properties of Sn-based 211 MAX phases

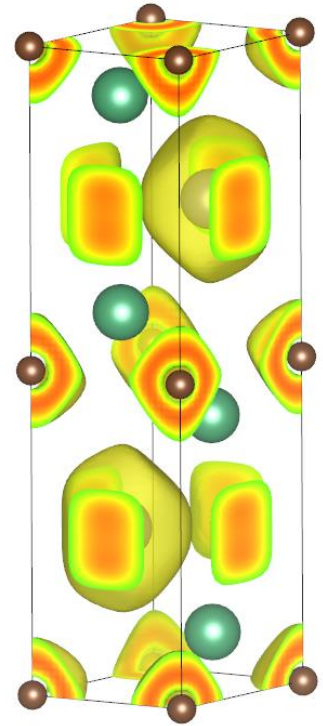
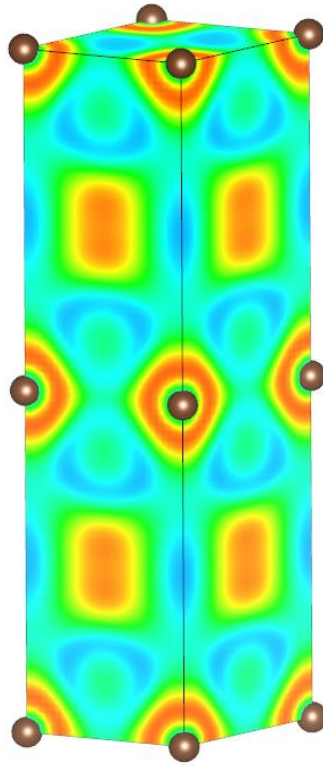
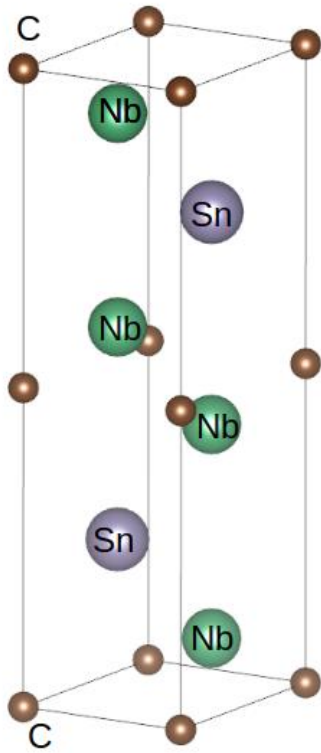
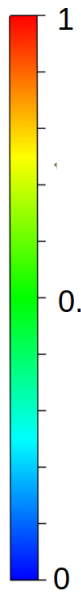
Optical properties	Polarization direction	Sn-based 211 MAX phases						
		Hf ₂ SnC	Lu ₂ SnC	Nb ₂ SnC	Sc ₂ SnC	Ti ₂ SnC	V ₂ SnC	Zr ₂ SnC
$\varepsilon_1(0)$	$\langle 100 \rangle$	-3204.2	-3438.3	-2957.8	-3431.3	-3396.5	-3259.6	-3409.4
	$\langle 001 \rangle$	-3352.4	-3437.1	-3369.5	-3434.4	-3407.8	-3294.2	-3411.9
$\varepsilon_2(0)$	$\langle 100 \rangle$	17393.4	17308.4	17491.7	17309.6	17319.1	17371.9	17315.2
	$\langle 001 \rangle$	17337.4	17308.5	17322.1	17310.1	17315.4	17349.5	17314.7
$n(0)$	$\langle 100 \rangle$	85.0936	84.2861	85.9716	84.3062	84.4172	84.8985	84.3750
	$\langle 001 \rangle$	84.5758	84.2894	84.4906	84.3004	84.3795	84.7503	84.3675
$k(0)$	$\langle 100 \rangle$	102.201	102.676	101.730	102.659	102.580	102.310	102.609
	$\langle 001 \rangle$	102.496	102.673	102.509	102.669	102.605	102.356	102.615
Average R in VLR	$\langle 100 \rangle$	0.50454	0.44843	0.50928	0.50452	0.50794	0.48653	0.49913
	$\langle 001 \rangle$	0.42451	0.42690	0.54128	0.41893	0.45616	0.52891	0.44115
$\sigma(0)$	$\langle 100 \rangle$	21.0282	20.9255	21.1472	20.9270	20.9384	21.0023	20.9338
	$\langle 001 \rangle$	20.9606	20.9257	20.9421	20.9275	20.9340	20.9752	20.9331
ω_p	$\langle 100 \rangle$	15.2277	15.5528	16.1857	11.0262	13.8616	15.1867	14.1741
	$\langle 001 \rangle$	15.8299	16.8209	16.5619	12.0754	13.9569	15.6564	14.5630
$\alpha(0)$	$\langle 100 \rangle$	16486.1	16562.7	16410.0	16559.9	16547.2	16503.6	16551.8
	$\langle 001 \rangle$	16533.7	16562.2	16535.7	16561.5	16551.1	16511.1	16552.8

Fig. S1

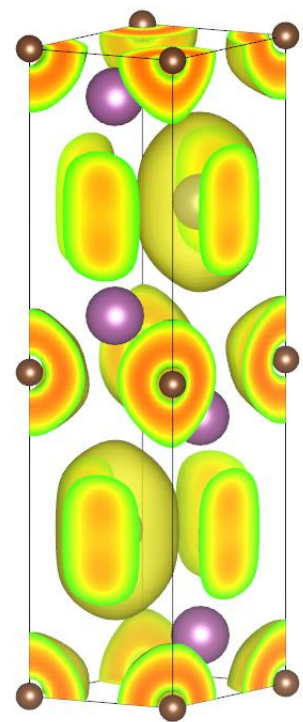
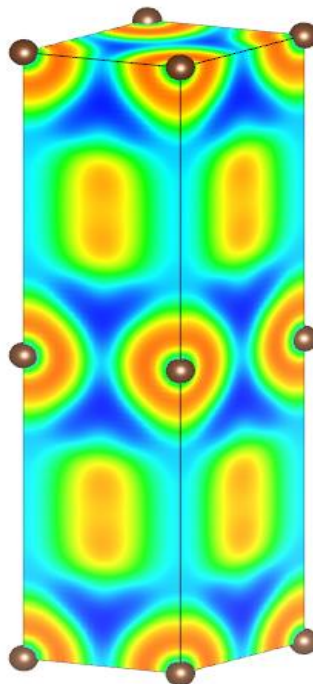
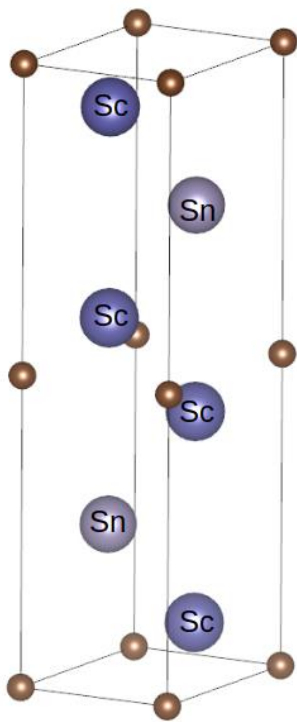
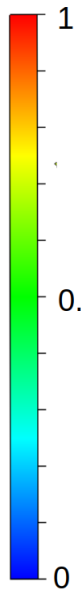
ELF function



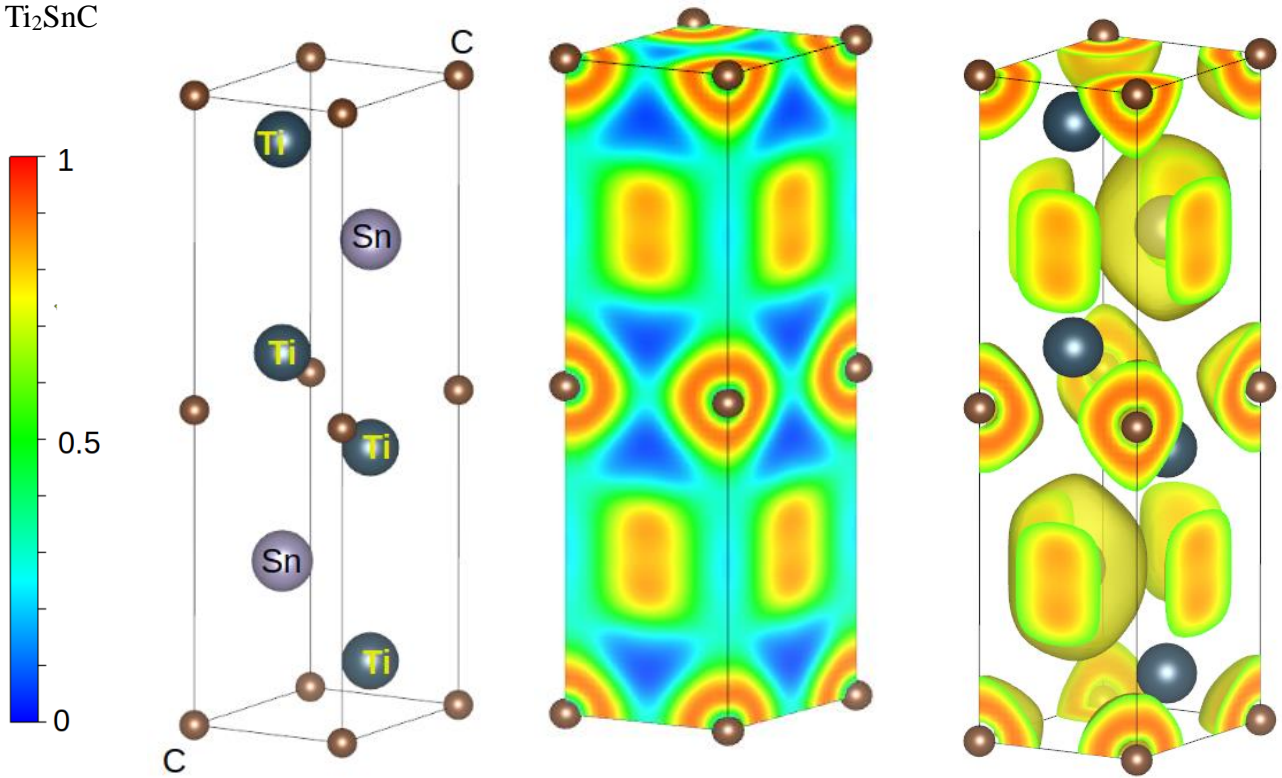
Nb_2SnC



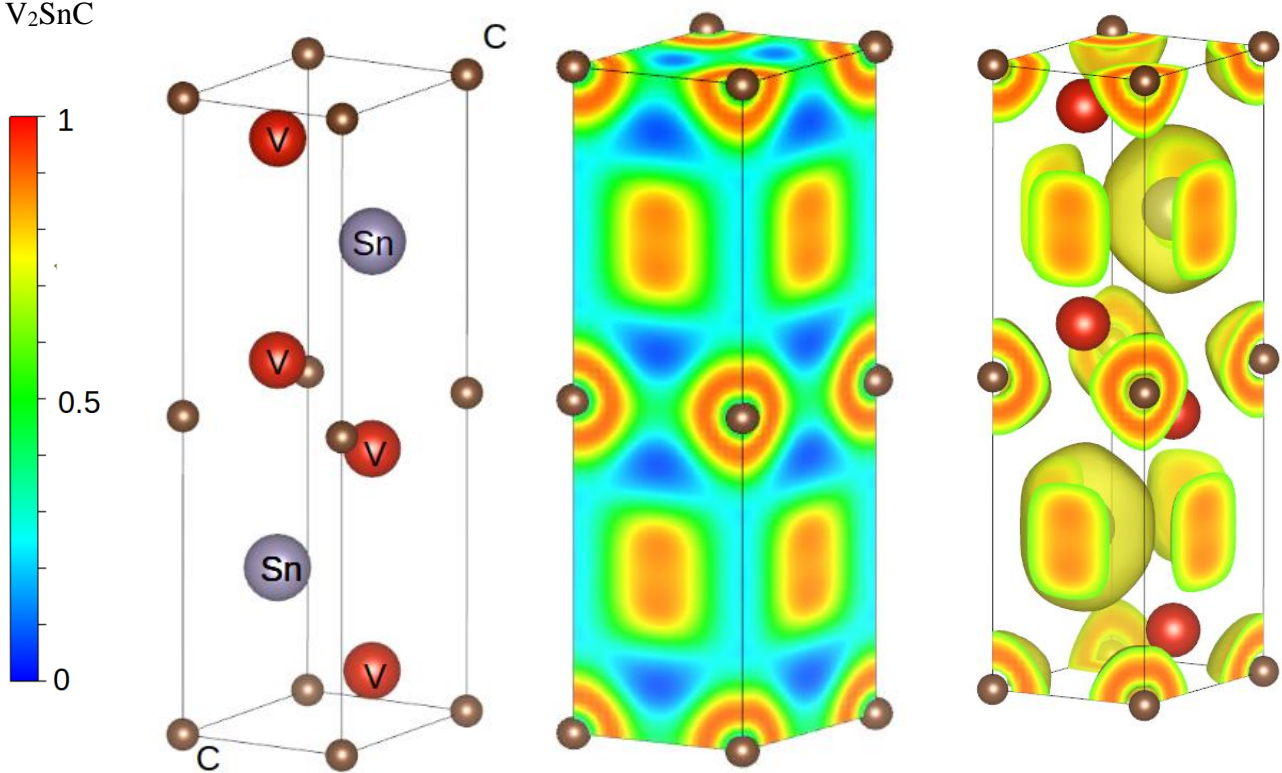
Sc_2SnC



Ti₂SnC



V₂SnC



Zr₂SnC

