Modulating the Framework Negative Charge Density in the System [BDT−TTP•+]/[Re6S5Cl91-]/[Re6(S/Se)6Cl82-]/[Re6S7Cl73-]

Titre	Modulating the Framework Negative Charge Density in the System [BDT−TTP•+]/[Re6S5Cl91-]/[Re6(S/Se)6Cl82-]/[Re6S7Cl73-]
Type de publication	Article de revue
Auteur	Perruchas, Sandrine [1], Boubekeur, Kamal [2], Canadell, Enric [3], Misaki, Yohji [4], Auban-Senzier, Pascale [5], Pasquier, Claude [6], Batail, Patrick [7]
Type	Article scientifique dans une revue à comité de lecture
Année	2008
Langue	Anglais
Date	2008/03
Numéro	11
Pagination	3335 - 3348
Volume	130
Titre de la revue	Journal of the American Chemical Society
ISSN	0002-7863
Résumé en anglais	A series of 2D metals, β-(BDT-TTP)6[Re6Se6Cl8]·(CHCl2−CHCl2)2, 2; β-(ST-TTP)6[Re6S6Cl8]·(CH2Cl−CHCl2)2, 3; β-(BDT-TTP)7[Re6S6Cl8]0.5[Re6S7Cl7]0.5·(CH2Cl2), 4; β-(BDT-TTP)7[Re6Se6Cl8]0.5[Re6S7Cl7]0.5·(CH2Cl2), 5; β-(BDT-TTP)8[Re6S7Cl7]·(CH2Cl2)4, 6 (BDT-TTP and ST-TTP are 2,5-bis(1,3-dithiol-2-ylidene)-1,3,4,6-tetrathiapentalene and 2-(1,3-diselenol-2-ylidene)-5(1,3-dithiol-2-ylidene)-1,3,4,6-tetrathiapentalene, respectively) is reported to have one single β-slab layered topology despite successive increases of the cluster anion negative charge. The charge density within the templating composite inorganic−neutral molecule slab is shown to remain above a threshold of ca. one negative charge per square nanometer, that is, for cluster anions with two negative charges and higher. Conversely, discrete stacks are shown to be stabilized instead in the semiconducting salts (BDT-TTP)2[Re6S5Cl9], 1 where the cluster anion bears one negative charge only. The electronic structure of salts 2−6 is shown to be very stable and kept almost intact across the series. The templating strategy is shown to fulfill its anticipated potential for deliberate installment of incommensurate band fillings in molecular metals. The deliberate admixture of the 6:1 and 8:1 structures yields novel phases with a 7:1 stoichiometry with the anticipated crystal and electronic structures. The action at the organic−inorganic interface triggered by changing the anion charge yet keeping its shape and volume identical, which ultimately governs the shape of the unit cell, is of paramount importance in defining the Fermi surface of these metallic salts. The present BDT-TTP salts thus provide a series of materials with strongly related but subtly different Fermi surfaces worthy of many physical studies. Shubnikov−de Haas measurements are expected to be particularly interesting since they are especially sensitive to the details of the Fermi surface.

Notes	Champ "Titre" tronqué, voir ci-dessous pour le titre complet: Modulating the Framework Negative Charge Density in the System [BDT−TTP•+]/[Re6S5Cl91-]/[Re6(S/Se)6Cl82-]/[Re6S7Cl73-]: Templating by Isosteric Cluster Anions of Identical Symmetry and Shape, Variations of Incommensurate Band Filling, and Electronic Structure in 2D Metals
URL de la notice	http://okina.univ-angers.fr/publications/ua2075 [8]
DOI	10.1021/ja074774s [9]
Lien vers le document	http://dx.doi.org/10.1021/ja074774s [9]

Liens

[1] http://okina.univ-angers.fr/publications?f[author]=2932
[2] http://okina.univ-angers.fr/publications?f[author]=2933
[3] http://okina.univ-angers.fr/publications?f[author]=2598
[4] http://okina.univ-angers.fr/publications?f[author]=2934
[5] http://okina.univ-angers.fr/publications?f[author]=2599
[6] http://okina.univ-angers.fr/publications?f[author]=2618
[7] http://okina.univ-angers.fr/patrick.batail/publications
[8] http://okina.univ-angers.fr/publications/ua2075
[9] http://dx.doi.org/10.1021/ja074774s