

parameters $a \approx 12.5$, $b \approx 6.2$, $c \approx 18.4$ Å, and $V \approx 1400$ Å³. Similar to the $LnNiSb_2$ compounds, these compounds are layered but consist of rare-earth atoms located above and below planes of nearly square, buckled Sb nets, however with layers of highly distorted edge- and face-sharing $NiSb_6$ octahedra. The structures of the $LnNi_xSb_2$ ($Ln = Y, Gd - Er$; $x \approx 0.6$) and $LnNiSb_3$ ($Ln = Pr, Nd, Sm$) compounds are similar to the structure of the simple binary phases $LnSb_2$ ($Ln = La-Nd, Sm, Gd-Er$). In an effort to correlate and elucidate the origin of the physical behavior observed, the structural units found within these three families will be compared.

Keywords: rare-earth, antimonides, single crystal

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The Crystal Growth and Structure and Property Relationships of Pr-Ni-Ga Phases

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Single crystals of two new ternary compounds, Pr_2NiGa_{10} and Pr_2NiGa_{12} were synthesized by flux methods. Single crystal X-ray diffraction data were collected and structures were solved for Pr_2NiGa_{10} and Pr_2NiGa_{12} . Pr_2NiGa_{10} , which crystallizes in a tetragonal space group $I4/mmm$, $Z = 2$, with the lattice parameters: $a = 4.2330$ (4) and $c = 26.364$ (3), $R_{\text{factor}} = 2.71\%$, was found to be isostructural to Ce_2PdGa_{10} .^[1] Pr_2NiGa_{12} , which crystallizes in tetragonal space group $P4/nbm$, $Z = 2$, with the lattice parameters: $a = 6.0080$ (7) and $c = 15.454$ (3), $R_{\text{factor}} = 4.2\%$, was found to be isostructural to Ce_2PdGa_{12} .^[2] The structure, transport, and magnetic properties of these compounds will be compared to other Ln_2PdGa_{10} ($Ln = La, Ce$) and Ln_2PdGa_{12} ($Ln = La, Ce$) phases.

[1] Millican J. N., Macaluso R. T., Young D. P., Moldovan M., Chan J. Y., *J. Solid State Chem.*, 2004, **177**, 4695-4700. [2] Macaluso R. T., Millican J. N., Lee H., Nakaatsuji S., Carter B., Nelson M., Fisk Z., Chan J.Y., 2005, *in preparation*.

Keywords: Pr-Ni-Ga phases, structural features, physical properties

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Structural Basis for the Diverse DNA Sequence Recognition by C/EBPβ Homodimer

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The CAAT-enhancer binding proteins (C/EBPs) are the bZIP family transcriptional regulatory factors, which play important roles during cell differentiation through regulating various gene expressions.

There are several kinds of the transcription factors belonging to the bZIP family such as c-Jun, Fos, CREB, etc, which recognize their specific DNA sequence as a homodimer or a heterodimer. In the case of a homodimer, the recognition sequences found in the native promoters are usually symmetric.

On the other hand, C/EBPs recognition sequences in the native promoters are mostly asymmetric even when C/EBPs, also belonging to the bZIP family, work as a homodimer, resulting in their much variety of target sequences.

To elucidate molecular mechanisms of C/EBPs for specific DNA recognition, we performed the structural analyses of several kinds of binary complexes composed of C/EBPβ, which is a member of C/EBPs, and various native promoter sequences or an artificial high affinity symmetric sequence, and the functional analyses such as a measurement of DNA binding affinity of C/EBPβ or its mutants designed from the structure using Surface Plasmon Resonance (SPR).

We could identify several conserved amino acids characteristic for C/EBPβ, which would play critical roles in its recognition of asymmetric DNA sequences.

Keywords: protein-DNA recognition, transcription factor, DNA-protein complexes

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Ab-initio Modeling of Electronic Transport Properties: a Structural Informer

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Functional materials often need to be structurally adjusted for optimizing their relevant properties. In the case of a thermoelectric (TE) material, the original atomic composition and structure is modified to enhance its figure of merit $Z \cdot T = T \cdot (S^2 \sigma / \kappa)$, where the Seebeck coefficient S , the electrical and thermal conductivity σ and κ are the material's transport properties. Doping is a common line of attack to optimize a TE material, and the relationship between the possible structural outcomes and the related transport properties, upon doping, may serve as a guidance to rationalize this empirical $Z \cdot T$ improvement procedure.

Recently [1] it has been shown that the *ab-initio* calculated electronic transport (ET) properties are useful *structural informers* for the doped semiconductor crystalline systems since these properties are rather sensitive to the location, the chemical nature and the concentration of the dopant atom. This fact establishes the *ab-initio* modeling as a particularly suited approach to assist the TE materials optimization.

The case of X-doped (X=Te, Sn, Fe, alkaline earth metal) $CoSb_3$ is as an interesting example of the ability of this approach to enlighten the effects the structural modifications have on a potentially highly performing TE material, especially when experiments are unable to recover detailed information on the geometric and electronic structure.

[1] Bertini L., Gatti C., *J. Chem. Phys.*, 2004, **121**, 8983.

Keywords: ab-initio calculations, crystal Structure, electronic transport properties

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Crystal Structures and Physical Properties of Flurbiprofen Salts

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Flurbiprofen is a nonsteroidal anti-inflammatory agent bearing a carboxyl group. As the free acid its aqueous solubility is only 0.03 mg mL⁻¹. Hydrophobicity of the counter ion does not fully determine the solubility of its amine salts[1], being 0.37, 2.80, 0.64 and 0.17 mg mL⁻¹ for the cyclohexyl(CH)-, hexyl-, octyl- and adamantyl(AD)-ammonium salts respectively. ΔH of fusion is 159.0 J g⁻¹ for the CH but only 81.0 J g⁻¹ for the hexylammonium salt.

We report structures of the stable CH and AD salts, acquired with synchrotron radiation because they exist as fine needles.

Crystal, T	a/Å	b/Å	c/Å	β/°	ρ/Mgm ⁻³
CH, 150K	14.7991	6.3014	19.7845	91.273	1.237
CH, 291K	15.0841	6.2988	19.8939	91.146	1.207
AD, 150K	39.350	6.3973	16.9976	90	1.228
AD, 291K	39.514	6.4257	17.1454	90	1.213

In both cases the cycloalkyl group covers the 2-fold disordered fluorophenyl ring, forming a clear hydrophobic domain. Hydrogen bonds join three ammonium H atoms to two carboxylate O atoms and create infinite ladders along the short b axis, which in CH shows no thermal expansion while the a axis expands by 1.9% over 141K.

[1] Anderson B.D., Conradi R.A., *J. Pharm. Sci.*, 1985, **74**, 815.

Keywords: solubility, thermal expansion, synchrotron radiation