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The decision to sporulate in *Bacillus subtilis* is primarily governed by the histidine kinase KinA instigating a phosphorelay resulting in the phosphorylation of the transcription factor Spo0A. The KipI protein is a regulator of this pathway, produced in response to low dietary nitrogen and high glucose conditions. KipI binds KinA, preventing the autophosphorylation required for the instigation of the phosphorelay. The KipA protein is expressed from the same operon as KipI and prevents its function as an inhibitor of KinA autokinase activity (an anti-anti-kinase). We have overexpressed and purified both proteins to homogeneity and demonstrated that they interact to form a complex. Biophysical investigation including small angle X-ray scattering and neutron contrast variation (using deuterated KipI) show that whilst the individual components are dimers at high concentration, when combined they form a 1:1 protein complex. The reconstructed shape of the KipI component closely resembles the structural envelope of a homologue ascribed as one subunit of an enzyme involved in urea metabolism – allophanate hydrolase. Although no structural model for KipA exists, at the amino acid level it resembles another allophanate hydrolase subunit, raising the question of the evolution and function of these ubiquitous folds. Implications as to how anti-anti-kinase activity is achieved are discussed.

Keywords: small-angle scattering, neutron contrast variation, signal transduction

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Synthesis, microstructure and catalytic property of nanocrystalline $\text{La}_{1-x}\text{Ce}_x\text{MnO}_3$

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Manganites have attracted much attention of many researchers due to their fascinating physical and chemical properties, including catalytic one. In this study, Ce- doped nanocrystalline $\text{La}_{1-x}\text{Ce}_x\text{MnO}_3$ ($x=0.05 - 0.2$) powders have been prepared using sol - gel method at a relatively (800°C). The crystal structure was examined by X-ray powder diffraction (XRD). The change in morphology, particle size and its surface area were also investigated by FE-SEM, TEM, SEM, BET measurements. Warren-Averbach and Williamson-Hall methods were used for microstructural analysis. The catalytic oxidation over hydrocarbon of nanopowders has been investigated.

Keywords: Ce-doped nanocrystalline LaMnO_3 , microstructure, catalytic property

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Site preference of Mn in Zn_2SiO_4 phosphor by combined Rietveld refinement

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$\text{Zn}_2\text{SiO}_4:\text{Mn}^{2+}$ as a green-color emitting phosphor which have an emission peak around 517 nm under UV excitation (247 nm) has been synthesized in solid state reaction. The combined Rietveld refinement was carried out to determine the site preference of Mn^{2+} ions in Zn_2SiO_4 phosphor. Of possible cation-disorder models, the best structural refinement result was obtained from a model that Mn^{2+} ions substitute for Zn^{2+} ions in ZnO_4 tetrahedra. The model proposed by the combined Rietveld refinement was corroborated by the first-principle pseudopotential calculation. The converged weighted *R*-factor, R_{wp} , and the goodness-of-fit indicator, S ($= R_{\text{wp}}/R_e$) were 9.17 % and 2.40, respectively. The occupancies of Mn^{2+} ions for two different Zn sites were 0.034(4) and 0.006(4), respectively. The refined model described a structure in space group *R3* (No. 148) with $Z = 18$, $a = b = 13.9611(1) \text{ \AA}$, $c = 9.3294(1) \text{ \AA}$ and $\gamma = 120^\circ$.

Keywords: phosphors, Rietveld analysis, X-ray neutron powder diffraction

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Ab initio structural characterization of $\text{Bi}_{10}\text{Mo}_3\text{O}_{24}$ by TEM, X-ray and neutron powder diffraction

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$\text{Bi}_2\text{O}_3\text{-MoO}_3$ system shows a full panoply of phases depending on Bi/Mo ratio. They present great interest because of their catalytic and ionic conductivity properties. Among them, for $x\text{Bi}_2\text{O}_3:\text{MoO}_3$ $1 < x < 2$ high temperature procedure for the chemical preparation yields mixtures, however single phases have been isolated by low T synthesis methods. In this sense we have characterized a new homologous series of oxides $\text{Bi}_{2(n+2)}\text{Mo}_n\text{O}_{6(n+1)}$ with $n=3,4,5$ and 6. For a deep understanding on the structure-property relationships there is a lack of crystallographic knowledge on these materials arising from the powder nature of the new obtained phases. Nevertheless, a multitechnique approach has been followed in order to solve their crystal structures. Electron diffraction patterns can be interpreted as a fluorite-type structure which gives rise to the basic lattice reflections, while weaker ones can be seen as satellites produced by a structural modulation. From HRTEM micrographs and using the metric relationship between the observed supercell and the basic fluorite one we infer cationic models for the new phases whose image simulations match well with the experimental images. We have used this cationic framework elucidation as starting point for the whole characterization of the structure by performing simultaneous Rietveld refinement of multipattern X-ray and neutron powder diffraction data, taking advantage of the neutron scattering length for O location. As example we show the simplest $\text{Bi}_{10}\text{Mo}_3\text{O}_{24}$ structure with 5Bi, 2Mo and 13 O different crystallographic positions in the asymmetric unit. It belongs to the monoclinic space group *C2* with $z=2$ and cell parameters: $a=23.7282(2) \text{ \AA}$, $b=5.64906(6) \text{ \AA}$, $c=8.68173(9) \text{ \AA}$, $\beta=95.8668(7)^\circ$. It shows very good agreement between observed and calculated patterns.

Keywords: *ab-initio* structure determination, neutron and X-ray scattering, oxides ionic conductors