Poster Presentation

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Mixed Alkaline Earth Germanides A2MGe2 (A= Ca/Sr; M= Sn,Pb)

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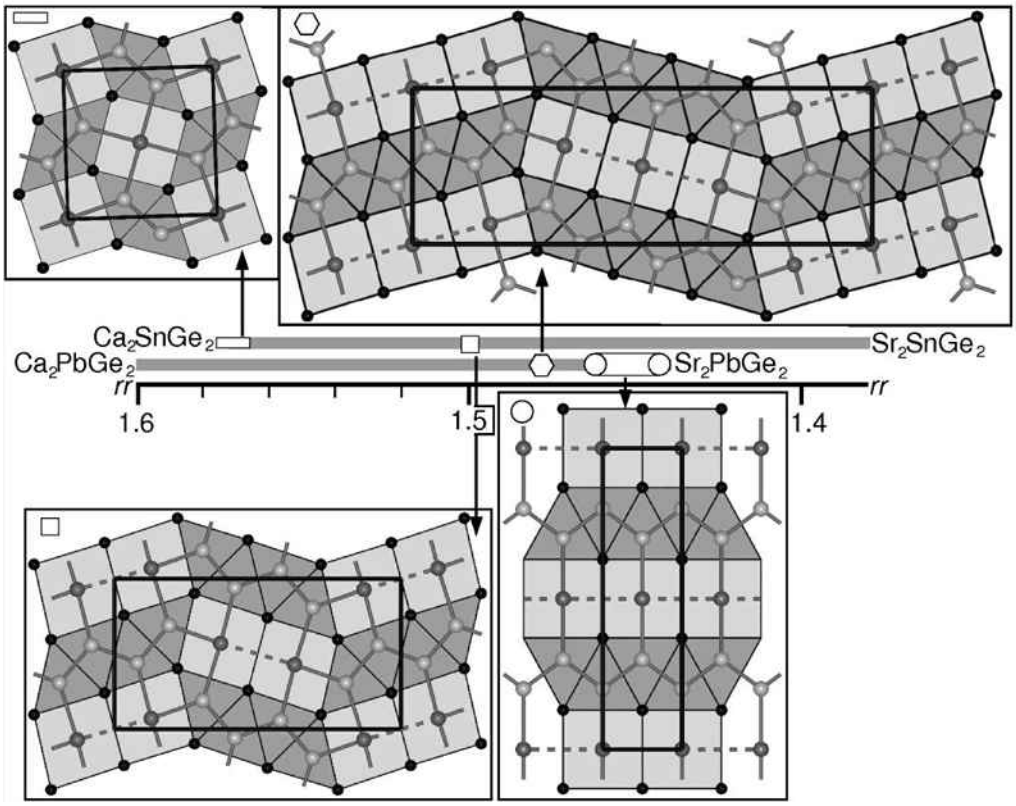
The crystal structures of the mixed alkaline earth tetrelides with the composition (CaxSr1-x)2MGe2 (M= Sn,Pb) exhibit identically stacked planes consisting of square planar coordinated M atoms (light gray) and [Ge]m zigzag chain pieces of varying lengths m. Each Ge atom is thereby coordinated by A atoms forming trigonal prisms (dark gray). The chain length m depends on the radius ratio rM4-/rA2+ (rr), whereat the M4- radius was estimated from the average Ca-M distances in the structures of Ca2M, which exhibit isolated tetrel anions. Depending on this radius ratio the structures of the title compounds feature [Ge]m chains of lengths m of 2, 4, 6 and infinite. Starting with Ge-Ge dumbbells in Ca2SnGe2 (rr= 1.57, space group P4/mbm, a= 748.58(13), c= 445.59)(8) pm, R1= 0.060, Mo2FeB2 type; cf. also Yb2SnGe2 [1], fig. top left), (Ca0.58Sr0.42)2SnGe2 shows Ge4 zigzag chain pieces (rr= 1.50, Pbam, a= 781.01(2), b= 1477.95(3), c= 457.00(1) pm, R1= 0.018, La2NiIn2 type; cf. also (Ca0.34Eu0.66)2PbGe2 [2], fig. bottom left). Ge6 pieces are present in (Ca0.23Sr0.77)2PbGe2 (rr= 1.48, Pbam, a= 2311.20(15), b= 791.64(5), c= 458.53(3) pm, R1= 0.073, new type, fig. top right) and infinit Ge chains in (CaxSr1-x)2PbGe2 (rr= 1.44-1.46, x= 0 to 0.22, Cmmm; for x= 0: a= 402.36(11), b= 1542.29(42), c= 463.27(10) pm, R1= 0.064, Mn2AlB2 type; cf. also (Sr0.21Eu0.79)2PbGe2 [2], fig. bottom right). In this series, i.e. with increasing m, the connectivity of M changes from a square planar coordination by four Ge in Ca2SnGe2 ([MGe4]) via [MGe3M] in (Ca0.58Sr0.42)2SnGe2 and [MGe3M]2[MGe2M2] in (Ca0.23Sr0.77)2PbGe2 up to [MGe2M2] in Sr2PbGe2, finally. The details of chemical bonding are discussed on the basis of band structure calculations.

[1] *M. Jehle, I. Dürr, S. Fink, B. Lang, C. Röhr, Acta Crystallogr., 2012, A68, 192.,* ***[2]*** *N.-T. Suen, J. Hooper, E. Zurek, S. Bobev, J. Am. Chem. Soc., 2012, 134, 12708-12716.*



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