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Design and discovery of a novel half-Heusler transparent hole conductor made of all-metallic heavy elements

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Transparent conductors combine two generally contradictory physical properties, but there are numerous applications where both functionalities are crucial. Previous searches focused on doping wide-gap metal oxides. Focusing instead on the family of 18 valence electron ternary ABX compounds that consist of elements A, B and X in 1:1:1 stoichiometry, we search

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(C)

15,

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)⁶.

(C

A-⁷, (n-) C A²⁸,

C₂⁹ (p-) C.

10

()

C

C

9,11 14

p-

()

()

()

(4 2.5)

()

(<0.5 0)

()

()

()

()

()

()

()

18-

AB

AⁿB¹⁰ (8-n)

A⁽ⁿ⁺¹⁾B⁹ (8-n) (n=1, 2, 3, 4)

1 5, 9 17

AB)

(

;

C . B

AB

483

18

AB

15,

400

83

16,17

18,19

()

AB

()

... AB (...)
A, C, ...)
A B

C A 2 : 0.46 $\sqrt{18^{-1} - 1}$, ... C 2 2), ...

24. ... Phys. Rev. **139**, A796–A823 (1965).
25. ... et al. A ... Nat. Mater. **9**, 559–564 (2010).
26. ... & ... B ... Z. Tech. Phys. **12**, 593–601 (1931).
27. A ... A ... J. Phys. D: Appl. Phys. **40**, 2210 (2007).
28. ... , C ... C, ... & ... 8 ... 220° ... J. Appl. Phys. **44**, 2917–2918 (1973).
29. ... B ... & ... Phys. Rev. Lett. **77**, 3865–3868 (1996).
30. ... & ... Phys. Rev. B **59**, 1758–1775 (1999).
31. ... B ... A ... C ... & ... A ... Phys. Rev. B **57**, 1505–1509 (1998).
32. ... & ... A. A ... Phys. Rev. B **78**, 235104 (2008).
33. ... & ... A ... Phys. Rev. Lett. **93**, 156404 (2004).
34. ... Mater. Res. Bull. **3**, 37–46 (1968).

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... A ... B ... C ... AC36-08 28308 ... C