Fl 52

MnS_2
FeS_2
CoS_2
NiS_2
Структура

1960

Elliott N.,

J. Chem. Phys., 1960, 33, 903

Межатомные расстояния в FeS_2, CoS_2 и NiS_2.

(+2)

	S-S (A)	M-S (A)
MnS_2	2,086	2,59
FeS_2	2,171	2,259
CoS_2	2,124	2,315
NiS_2	2,065	2,396

61008.9027
Ph, Ch, TC, MGU

54969 FeS_2 (син. носи)

1976

ЖЧ 14717

Lutz H.D., Willich P., Haeuseler H. Gitterschwingungsspektren. XVII. Kraftkonstanten- und Normalkoordinatenrechnungen an Übergangsmetall-Dichalgeniden und -Diphosphiden mit Pyritstruktur. "Z.Naturforsch.",1976,31a,N7,847-852 (нем.,рез.англ.)

689 691   0719 ВИНИТИ

FeS_2

1976

Ishii Motoliko

Бумозке. 1976, N19, 450-5

(синт. к.р.)

(см. TiO_2; III)

FeS_2

1983

100: 27599x **Complete first-order Raman spectra of the pyrite structure compounds iron disulfide, manganese disulfide, and silicon diphosphide.** Vogt, H.; Chattopadhyay, T.; Stolz, H. J. (Max-Planck-Inst. Festkoerperschung, 7000 Stuttgart, Fed. Rep. Ger.). *J. Phys. Chem. Solids* 1983, 44(9), 869-73 (Eng). The 1st-order Raman spectra of FeS_2, MnS_2, and SiP_2 were measured at room temp. The frequencies of all Raman-active phonons were obtained. The displacement patterns are described and the extent to which the concept of the mol. crystal can be applied is discussed.

(CKP)

(42)

C.A. 1984, 100, N4

FeS_2

1984

1 Б2244. Расчеты электронной структуры, фотоэлектронные спектры, оптические спектры и мессбауэровские параметры для пиритов MS_2 (M=Fe, Co, Ni, Cu, Zn). Electronic-structure calculations, photoelectron spectra, optictal spectra, and Mössbauer parameters for the pyrites MS_2 (M=Fe, Co, Ni, Cu, Zn). Lauer S., Trautwein A. X., Harris F. E. «Phys. Rev. B: Condens. Matter», 1984, 29, № 12, 6774—6783 (англ.)

В кластерной модели для дисульфидов переходных металлов MS_2 с M=Fe, Co, Ni, Cu, Zn и структурой типа пирита проведены расчеты электронного строения

расчет электрон. спектров

CoS_2, NiS_2, CuS_2, ZnS_2

(Н) ⊗

Х. 1985, 19, N1

в приближении сильной связи. Рассчитаны фотоэлектронные спектры, оптич. х-ки и тензор градиента эл. поля. Сходимость итерац. процесса достигалась при кластере размером не меньше, чем $[M(S_2)_6]^{10-}$. Расчеты позволили осуществить отнесение линий в измеренных спектрах. Установлено также, что знак константы ядерного с квадрупольного взаимодействия отрицателен для всех соединений, кроме ZnS_2. Оценены вклады в тензор градиента эл. поля от различных электронных оболочек и от решетки кристалла. На основании расчетных данных рассмотрен вопрос об интерпретации мессбауэровских спектров.

В. Г. Цирельсон

FeS_2 (K)

1998

states in polycryst. Si.

128: 313106f **Electronic structure of FeS_2: The crucial role of electron–lattice interaction.** Eyert, V.; Hock, K.–H.; Fiechter, S.; Tributsch, H. (Hahn–Meitner–Institut, Theory Department, Glienicker Strasse 100, D–14109 Berlin, Germany). *Phys. Rev. B: Condens. Matter Mater. Phys.* **1998**, 57(11), 6350–6359 (Eng), American Physical Society. Using the results of fully self–consistent all–electron 1st–principles calcns. for semiconducting Fe pyrite the authors discuss the major factors governing the semiconducting properties as well as the chem. bonding of this material. The calcns. are based on d. functional theory within the local d. approxn. and employ the augmented spherical wave method in its scalar–relativistic implementation. The electronic properties are dominated by strongly hybridized Fe 3d and S 3p states. The chem.

Н. спин мура

bonding is analyzed using an ab initio implementation of the crystal orbital overlap population. Chem. stability results mainly from the Fe–S bonding. While the upper part of the valence band is formed mainly from Fe $3dt_{2g}$–derived states the conduction band comprises the e_g–derived levels. The conduction band min., in contrast, is exclusively due to S 3p states, this fact explaining the obsd. high optical absorption. For the same reason the optical properties are strongly influenced by the short S–S bonds. Only small deviations in the S pair bond lengths involve rather drastic changes of the near–gap electronic states which might even turn the indirect band gap into a direct 1. These findings allow one to understand the rather high sensitivity of the optical band gap to the incorporation of defects. Finally, results open perspectives for photovoltaic applications of FeS_2.

CA 1998, 128, N25

1999

F: FeS2+
P: 3
131:162029 On the Structural Dichotomy of Cationic, Anionic, and Neutral Schroeder, Detlef; Kretzschmar, Ilona; Schwarz, Helmut; Rue, Chad; Armentrout, P. B. (Institut fuer Organische Chemie, Technischen Universit Berlin, Berlin D-10623, Germany). Inorg. Chem., 38(15), 3474-3480 (Engli 1999 Structural and thermochem. aspects of the FeS2+ cation are examd. by different mass spectrometric methods and ab initio calcns. using d. funct theory. Accurate threshold measurements provide thermochem. data for FeS FeS2+, and FeCS+, i.e., D0(Fe+-S) = 3.06 .+-. 0.06 eV, D0(SFe+-S) = 3.59 0.12 eV, D0(Fe+-S2) = 2.31 .+-. 0.12 eV, and D0(Fe+-CS) = 2.40

.+-. 0.12 Fortunate circumstances allow a refinement of the data for FeS+ by means ion/mol. equil., and the resulting D0(Fe+-S) = 3.08 .+-. 0.04 eV is among most precisely known binding energies of transition-metal compds. The pr results agree with previous exptl. findings and also corroborate the comp data for FeS+ and FeS2+. Ab initio calcns. predict a sextet ground state for FeS2+ with a cyclic structure. The presence of S-S and Fe-S bonds ac for the fact that not only reactions involving the disulfur unit but also sulfur-atom transfer can occur. In contrast, the FeS2- anion is an acycl disulfide. In the gas phase, neutral FeS2 may adopt either acyclic or cy structures, which are rather close in energy according to the calcns.

FeS_2^*
FeS_2^+

Om. 40035

1999

Detlef Schröder et al.,

Do, cmp-pa

Inorg. Chem. 1999, 38, 3474-3480

On the Structural Dichotomy of Cationic, Anionic, and

Neutral FeS_2.

Fe3+ | Om. 40840 | 2081

John Husband, Fernando Aguirre et al.,

Chem. Phys. Lett., 2001,

342, 75-84.

Photodissociation spectra

% transition metal sulfides: spin-orbit structure in charge transfer bands % FeS^+ and NiS^+.

F_2 I_2 $^{-101+12+}$ Ом. 41230 2002

Немцов. соавт.

Olaf Hübner and Joachim Sauer,

J. Chem. Phys., 2002, 116, N 2, 617–628

Dm · 41598

2002

$D_0(Fe_n^+ - S)$
$n = 2-5$

$D_0(SFe_{n-1}^+ - Fe)$
$n = 2-5$

$D_0(S_2Fe_{n-1}^+ - Fe)$
$n = 2,3$

Konrad Koszinowski
et al.,

J. Chem. Phys.,
2002, 117, N22,
10039 – 10056.