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类锂硅离子能级结构及软 X 射线激光光谱理论计算

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提　　要

本文采用 Hartree-Fock 自洽场方法，从理论上计算出类锂硅离子 $1s^2nl(n=2\sim7, l=0\sim5)$ 各能级能量，并给出在极紫外(波长小于 400Å)范围内各跃迁谱线的光谱性质、波长、振子强度和跃迁几率。对实验中已实现软 X 射线激光的跃迁(5*d*-3*p*, 5*f*-3*d*, 6*d*-3*p*, 6*f*-3*d*)，计算所得的跃迁波长与实验值完全相符。与现有文献的波长比较，相对误差不超过 1%。

关键词：类锂硅离子，软 X 射线激光光谱。

一、引　　言

近年来，以激光等离子体为增益介质实现软 X 射线激光取得了长足的进展[1]，已经越来越受到人们的重视。离子复合泵浦是实现 X 射线激光的主要物理机制之一[2~4]，它使得在较小规模的驱动激光装置上实现自发发射放大成为可能。最近，我们首次在 LF12# 激光装置上实现了类锂硅离子(Li-like Si XII) 5*f*-3*d*(88.9Å)，5*d*-3*p*(87.3Å)，(激光增益系数 G 为 $1.5\sim2.0\ \mathrm{cm^{-1}}$)和 6*f*-3*d*(75.8Å)，6*d*-3*p*(74.6Å)跃迁的软 X 射线激光($G\sim1.0\ \mathrm{cm^{-1}}$)，其激光驱动功率密度仅为 $2.5\times10^{12}\ \mathrm{W/cm^2}$。软 X 射线激光进一步向"水窗"(43.8～23.3Å)靠拢了[5,6]。

这一成果，使得理论上考察原子能级结构和光谱性质显得十分重要和迫切。在此之前，人们一般采用半经验公式，如瑞典的 Edlén 和西北师范学院王永昌等[7,8]。纯理论计算工作，吉林大学原子与分子物理研究所的朱颀人等作过一些探讨，并给出了 Si XII 5*f*-3*d* 及 5*d*-3*p* 跃迁的理论计算结果[9]。但是，Li-like XII 能级纯理论计算至今仍还不全面和系统，对软 X 射线激光跃迁的光谱性质的计算与讨论也很欠缺，特别是 6*f*-3*d*, 6*d*-3*p* (实验已实现激光输出的跃迁)以及实验工作者感兴趣的 7*f*-3*d*, 7*d*-3*p* 跃迁，光谱性质的理论数据至今未见报道。

本文以美国 Los Alamos 国家实验室提供的先进大型原子结构及光谱计算程序[10]，采用 Hartree-Fock 自洽场方程[11]，进行了原子结构的纯理论计算，首次给出了类锂硅离子($1s^2$ 封闭壳层及外层一电子的三电子系统)$1s^2nl(n=2\sim7, l=0\sim5)$各能级平均能量值，以及在极紫外(波长小于 400Å)波段跃迁谱线的光谱性质：波长、跃迁几率和振子强度等。其中，对已实验发现软 X 射线激光输出的跃迁 5*f*-3*d*, 5*d*-3*p*, 6*f*-3*d* 及 6*d*-3*p*，计算所得的

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跃迁波长与实验输出值很好相符。所提供的数据为今后进一步实验和理论分析了依据，对软X射线激光的实验研究也有着重要的指导意义。

二、能级结构的理论计算

本文以Los Alamos的计算程序，采用Hartree-Fock自洽场方法，进行了原子结构和纯理论计算。这个程序包括三个部分：RCN 34，RCN 2及RCG 9。其中：

RCN 34为用自洽场方法求解Hartree-Fock方程，考虑相对论修正和Breit修正等，从而得出原子或离子状态下各电子轨道的径向波函数及积分参量。

RCN 2为求解存在相互作用的组态之间的积分参量。

RCG 9为求解多组态的哈密顿矩阵，从而得出原子或离子组态的能级能量值，本征函数以及振子强度等*。

对原子结构纯理论计算，除了求解多组态Hartree-Fock方程或其相对论变型Dirac-Hartree-Fock方程外，还必须考虑其它一些效应的影响，以提高计算精度。一般说来有相对论效应，电子间的相关效应，核大小效应，Breit效应以及量子电动力学效应。

相对论效应来自两个方面：第一，在核附近的高速电子质量相对增加，由此使这些电子的平均轨道半径减小；第二，在核附近电子电荷密度的增加对核电荷产生额外的屏蔽效应，

Table 1 Si XII $1s^2\ nl(n=2\sim7,\ l=0\sim5)$ Average energy of evergy cnergy level

(unit: 1000 cm^{-1}=0.12eV)

No.	eney level ($1S^2nl$)	energy
1	2s	0
2	2p	197.909
3	3s	2393.756
4	3p	2448.352
5	3d	2468.177
6	3s	3207.427
7	4p	3229.866
8	4d	3238.215
9	4f	3239.274
10	5s	3578.853
11	5p	3590.192
12	5d	3594.454
13	5f	3594.961
14	5g	3595.160
15	6s	3778.943
16	6p	3785.450
17	6d	3787.910
18	6f	3788.197
19	6g	3788.314
20	6h	3788.348
21	7s	3898.910
22	7p	3902.987
23	7d	3904.534
24	7f	3904.787
25	7g	3904.712
26	7h	3904.810

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* 上述程序流程框图见文献[11]。

由此使外层电子的轨道半径增大。Cowan[11] 对该效应有较详细的描述，并给出了它对能量的修正公式。

电子间的相关效应即指电子-电子的库仑相关对能量的影响[11]。

一般都把原子核忽略其尺度，认为其库仑势函数类似于点电荷的势函数。但实际上除了最轻的元素外，为了更精确起见，必须考虑到原子核是有一定大小的，可被看作是均匀的带电球体或具有双参数费米分布。这就是核大小效应所考虑的修正。

Breit 效应包括磁和延迟效应的作用。它是考虑到单光子交换的静电库仑相互作用的动力学修正，这点可以通过在计算中增加一阶微扰形式的 Breit 算符来实现。

量子电动力学修正包括自能和真空极化两部分。它们均引起能级的量子电动力学拉姆(Lamb)漂移。这种修正在计算内次壳层束缚能时必须考虑，但我们计算类锂硅离子则可忽略。

计算是类锂硅离子的最低能态 $1s^2 2s$ 作为能级零点，把有关组态 $1s^2 nl(2\leqslant n\leqslant 7)\,^2L_j$ 一并输入，得到各能级平均能量如表 1 所示。此数据可作为估算各能级间跃迁波长的理论值。

三、类锂硅离子光谱性质数据

在表 2 中给出了类锂硅离子 $1s^2 nl(2\leqslant n\leqslant l)\,^2L_j$ 能级之间所有波长小于 400Å 的跃迁谱线的光谱性质：波长、振子强度和跃迁几率，以波长减小的顺序排列。计算中未考虑任何经验修正。

Table 2　Calcuated wavelengths, radiative transition probabilities and line strengths in Si for transitions of the type $1s^2n'l'^2L'_j\leftarrow 1s^2nl^2L_j$

transition $n'l'^2L'_j\leftarrow nl^2L_j$		wavelangth λ(Å)	oscillator strength gf(au)	transition probabilities gA(sec^{-1})
$5d\,^2D_{3/2}$	$7p\,^2P_{1/2}$	324.1434	0.0398	2.526E+09
$5d\,^2D_{5/2}$	$7p\,^2P_{3/2}$	324.1168	0.0716	4.548E+09
$5d\,^2P_{3/2}$	$7s\,^2S_{1/2}$	324.0997	0.0928	5 893E+09
$5d\,^2D_{3/2}$	$7p\,^2P_{3/2}$	323.9474	0.0080	5.061E+08
$5p\,^2P_{1/2}$	$7s\,^2S_{1/2}$	323.5618	0.0465	2.961E+09
$5g\,^2G_{9/2}$	$7f\,^2F_{7/2}$	323.0574	0.0117	7.503E+08
$5f\,^2F_{7/2}$	$7d\,^2D_{5/2}$	323.0386	0.0358	2.290E+09
$5g\,^2G_{7/2}$	$7f\,^2F_{5/2}$	323.0364	0.0091	5.789E+08
$5f\,^2F_{5/2}$	$7d\,^2D_{3/2}$	323.0145	0.0251	1.603E+09
$5g\,^2G_{7/2}$	$7f\,^2F_{7/2}$	323.0058	0.0003	2.145E+07
$5g\,^2G_{9/2}$	$7h\,^2H_{9/2}$	322.9756	0.0367	2.346E+09
$5g\,^2G_{9/2}$	$7h\,^2H_{11/2}$	322.9630	1.9812	1.267E+11
$5f\,^2F_{5/2}$	$7d\,^2D_{5/2}$	322.9535	0.0018	1.146E+08
$5g\,^2G_{7/2}$	$7h\,^2H_{9/2}$	322.9240	1.6145	1.033E+11
$5f\,^2F_{7/2}$	$7g\,^2G_{7/2}$	322.8095	0.0509	3.255E+09
$5f\,^2F_{7/2}$	$7g\,^2G_{9/2}$	322.7907	1.7800	1.139E+11
$5f\,^2F_{5/2}$	$7g\,^2G_{7/2}$	322.7245	1.3734	8.795E+10

(Continued)

transition $n'l'^2L'_j \leftarrow nl^2L_j$		wavelangth λ(Å)	oscillator stiength strength gf(au)	transition probabilities gA(sec^{-1})
$5d\ ^2D_{5/2}$	$7f\ ^2F_{5/2}$	322.3963	0.0562	$3.608E+09$
$5d\ ^2D_{5/2}$	$7f\ ^2F_{7/2}$	322.3657	1.1247	$7.218E+10$
$5d\ ^2D_{3/2}$	$7f\ ^2F_{5/2}$	322.2287	0.7876	$5.059E+10$
$5p\ ^2P_{3/2}$	$7d\ ^2D_{3/2}$	318.3340	0.0599	$3.944E+09$
$5p\ ^2P_{3/2}$	$7d\ ^2D_{5/2}$	318.2747	0.5395	$3.552E+10$
$5p\ ^2P_{1/2}$	$7d\ ^2D_{3/2}$	317.8150	0.3001	$1.982E+10$
$5s\ ^2S_{1/2}$	$7p\ ^2P_{1/2}$	308.6332	0.0838	$5.866E+09$
$5s\ ^2S_{1/2}$	$7p\ ^2P_{3/2}$	308.4556	0.1677	$1.175E+10$
$4p\ ^2P_{3/2}$	$5s\ ^2S_{1/2}$	286.8189	0.3042	$2.446E+10$
$4p\ ^2P_{1/2}$	$5s\ ^2S_{1/2}$	285.9960	0.1525	$1.244E+10$
$4d\ ^2D_{3/2}$	$5p\ ^2P_{1/2}$	284.2327	0.1107	$9.143E+09$
$4d\ ^2D_{5/2}$	$5p\ ^2P_{3/2}$	284.0723	0.1995	$1.649E+10$
$4d\ ^2D_{3/2}$	$5p\ ^2P_{3/2}$	283.8189	0.0222	$1.837E+09$
$4f\ ^2F_{5/2}$	$5d\ ^2D_{3/2}$	281.5531	0.0502	$4.226E+09$
$4f\ ^2F_{7/2}$	$5d\ ^2D_{5/2}$	281.5504	0.0718	$6.037E+09$
$4f\ ^2F_{5/2}$	$5d\ ^2D_{5/2}$	281.4253	0.0036	$3.023E+08$
$4f\ ^2F_{7/2}$	$5g\ ^2G_{7/2}$	281.0639	0.2993	$2.527E+10$
$4f\ ^2F_{7/2}$	$5g\ ^2G_{9/2}$	281.0248	10.4755	$8.847E+11$
$4f\ ^2F_{5/2}$	$5g\ ^2G_{7/2}$	280.9393	8.0835	$6.831E+11$
$4d\ ^2D_{5/2}$	$5f\ ^2F_{5/2}$	280.4459	0.2542	$2.156E+10$
$4d\ ^2D_{5/2}$	$5f\ ^2F_{7/2}$	280.3818	5.0858	$4.315E+11$
$4d\ ^2D_{3/2}$	$5f\ ^2F_{5/2}$	280.1990	3.5624	$3.026E+11$
$4p\ ^2P_{3/2}$	$5d\ ^2D_{3/2}$	274.6078	0.2264	$2.002E+10$
$4p\ ^2P_{3/2}$	$5d\ ^2D_{5/2}$	274.4862	2.0382	$1.804E+11$
$4p\ ^2P_{1/2}$	$5d\ ^2D_{3/2}$	273.8533	1.1350	$1.009E+11$
$4s\ ^2S_{1/2}$	$5p\ ^2P_{1/2}$	261.4903	0.2726	$2.659E+10$
$4s\ ^2S_{1/2}$	$5p\ ^2P_{3/2}$	261.1400	0.5459	$5.339E+10$
$4d\ ^2D_{5/2}$	$6p\ ^2P_{3/2}$	182.7458	0.0410	$8.189E+09$
$4d\ ^2D_{3/2}$	$6p\ ^2P_{1/2}$	182.7399	0.0228	$4.550E+09$
$4d\ ^2D_{3/2}$	$6p\ ^2P_{3/2}$	182.6409	0.0046	$9.115E+08$
$4f\ ^2F_{7/2}$	$6d\ ^2D_{5/2}$	182.2803	0.0128	$2.571E+09$
$4f\ ^2F_{5/2}$	$6d\ ^2D_{3/2}$	182.2589	0.0090	$1.800E+09$
$4p\ ^2P_{3/2}$	$6s\ ^2S_{1/2}$	182.2350	0.0663	$1.332E+10$
$6d\ ^2D_{5/2}$	$4f\ ^2F_{5/2}$	182.2279	0.0006	$1.287E+08$
$4f\ ^2F_{7/2}$	$6g\ ^2G_{7/2}$	182.1637	0.0405	$8.149E+09$
$4f\ ^2F_{7/2}$	$6g\ ^2G_{9/2}$	182.1543	1.4191	$2.853E+11$
$4f\ ^2F_{5/2}$	$6g\ ^2G_{7/2}$	182.1114	1.0950	$2.202E+11$
$4p\ ^2P_{1/2}$	$6s\ ^2S_{1/2}$	181.9025	0.0332	$6.697E+09$
$4d\ ^2D_{5/2}$	$6f\ ^2F_{5/2}$	181.8745	0.0533	$1.074E+10$
$4d\ ^2D_{5/2}$	$6f\ ^2F_{7/2}$	181.8590	1.0651	$2.148E+11$
$4d\ ^2D_{3/2}$	$6f\ ^2F_{5/2}$	181.7706	0.7459	$1.506E+11$
$4p\ ^2P_{3/2}$	$6d\ ^2D_{3/2}$	179.3230	0.0573	$1.188E+10$
$4p\ ^2P_{3/2}$	$6d\ ^2D_{5/2}$	179.2930	0.5154	$1.069E+11$
$4p\ ^2P_{1/2}$	$6d\ ^2D_{3/2}$	179.0010	0.2868	$5.970E+10$
$4s\ ^2S_{1/2}$	$6p\ ^2P_{1/2}$	173.0628	0.0756	$1.684E+10$

(Continued)

transition $nl'^2L'_j \leftarrow nl^2L_j$		wavelangth λ(Å)	oscillator strength gf(au)	transition probabilities gA(sec^{-1})
$4s\ ^2S_{1/2}$	$6p\ ^2P_{3/2}$	172.9740	0.1513	$3.372E+10$
$4d\ ^2D_{5/2}$	$7p\ ^2P_{3/2}$	150.4418	0.0159	$4.683E+09$
$4d\ ^2D_{3/2}$	$7p\ ^2P_{1/2}$	150.4130	0.0088	$2.603E+09$
$4d\ ^2D_{3/2}$	$7p\ ^2P_{3/2}$	150.3708	0.0018	$5.211E+08$
$4f\ ^2F_{7/2}$	$7d\ ^2D_{5/2}$	150.3272	0.0046	$1.348E+09$
$4f\ ^2F_{5/2}$	$7d\ ^2D_{3/2}$	150.3048	0.0032	$9.443E+08$
$4f\ ^2F_{5/2}$	$7d\ ^2D_{5/2}$	150.2916	0.0002	$6.747E+07$
$4f\ ^2F_{7/2}$	$7g\ ^2G_{7/2}$	150.2776	0.0130	$3.833E+09$
$4f\ ^2F_{7/2}$	$7g\ ^2G_{9/2}$	150.2735	0.4543	$1.342E+11$
$4f\ ^2F_{5/2}$	$7g\ ^2G_{7/2}$	150.2420	0.3505	$1.036E+11$
$4d\ ^2D_{5/2}$	$7f\ ^2F_{5/2}$	150.0701	0.0207	$6.125E+09$
$4d\ ^2D_{5/2}$	$7f\ ^2F_{7/2}$	150.0635	0.4136	$1.225E+11$
$4d\ ^2D_{3/2}$	$7f\ ^2F_{5/2}$	149.9994	0.2897	$8.587E+10$
$4p\ ^2P_{3/2}$	$7s\ ^2S_{1/2}$	149.5418	0.0268	$8.000E+09$
$4p\ ^2P_{1/2}$	$7s\ ^2S_{1/2}$	149.3178	0.0134	$4.018E+09$
$4p\ ^2P_{3/2}$	$7d\ ^2D_{3/2}$	148.3024	0.0245	$7.418E+09$
$4p\ ^2P_{3/2}$	$7d\ ^2D_{5/2}$	148.2896	0.2202	$6.678E+10$
$4p\ ^2P_{1/2}$	$7d\ ^2D_{3/2}$	148.0821	0.1225	$3.726E+10$
$4s\ ^2S_{1/2}$	$7p\ ^2P_{1/2}$	143.7948	0.0337	$1.087E+10$
$4s\ ^2S_{1/2}$	$7p\ ^2P_{3/2}$	143.7562	0.0674	$2.176E+10$
$3p\ ^2P_{3/1}$	$4s\ ^2S_{1/2}$	131.8774	0.1890	$7.250E+10$
$3p\ ^2P_{1/2}$	$4s\ ^2S_{1/2}$	131.4643	0.0948	$3.659E+10$
$3d\ ^2D_{3/2}$	$4p\ ^2P_{1/2}$	131.3253	0.0447	$1.727E+10$
$3d\ ^2D_{5/2}$	$4p\ ^2P_{3/2}$	131.2808	0.0804	$3.113E+10$
$3d\ ^2D_{3/2}$	$4p\ ^2P_{3/2}$	131.1525	0.0089	$3.469E+09$
$3d\ ^2D_{5/2}$	$4f\ ^2F_{5/2}$	129.7507	0.2911	$1.153E+11$
$3d\ ^2D_{5/2}$	$4f\ ^2F_{7/2}$	129.7241	5.8240	$2.308E+12$
$3d\ ^2D_{3/2}$	$4f\ ^2F_{5/2}$	129.6253	4.0799	$1.619E+12$
$3p\ ^2P_{3/2}$	$4d\ ^2D_{3/2}$	126.7621	0.2332	$9.679E+10$
$3p\ ^2P_{3/2}$	$4d\ ^2D_{5/2}$	126.7116	2.0995	$8.722E+11$
$3p\ ^2P_{1/2}$	$4d\ ^2D_{3/2}$	126.3804	1.1695	$4.884E+11$
$3s\ ^2S_{1/2}$	$4p\ ^2P_{1/2}$	119.6971	0.0000	$0.000E+00$
$3s\ ^2S_{1/2}$	$4p\ ^2P_{3/2}$	119.5536	0.0000	$0.000E+00$
$3d\ ^2D_{5/2}$	$5p\ ^2P_{3/2}$	89.1354	0.0159	$1.332E+10$
$3d\ ^2D_{3/2}$	$5p\ ^2P_{1/2}$	89.1170	0.0088	$7.404E+09$
$3d\ ^2D_{3/2}$	$5p\ ^2P_{3/2}$	89.0763	0.0018	$1.483E+09$
$3d\ ^2D_{5/2}$	$5f\ ^2F_{5/2}$	88.7752	0.0449	$3.798E+10$
$3d\ ^2D_{5/2}$	$5f\ ^2F_{7/2}$	88.7688	0.8976	$7.598E+11$
$3d\ ^2D_{3/2}$	$5f\ ^2F_{5/2}$	88.7165	0.6287	$5.328E+11$
$3p\ ^2P_{3/2}$	$5s\ ^2S_{1/2}$	88.5186	0.0407	$3.468E+10$
$3p\ ^2P_{1/2}$	$5s\ ^2S_{1/2}$	88.3323	0.0204	$1.745E+10$
$3p\ ^2P_{3/2}$	$5d\ ^2D_{3/2}$	87.3202	0.0546	$4.773E+10$
$3p\ ^2P_{3/2}$	$5d\ ^2D_{5/2}$	87.3079	0.4912	$4.298E+11$
$3p\ ^2P_{1/2}$	$5d\ ^2D_{3/2}$	87.1389	0.2734	$2.402E+11$
$3s\ ^2S_{1/2}$	$5p\ ^2P_{2/1}$	83.6055	0.4899	$4.675E+11$

(Continued)

transition $n'l'^2L'_j\leftarrow nl^2L_j$		wavelangth $\lambda(\text{Å})$	oscillator strength gf(au)	transition probabilities $gA(\sec^{-1})$
$3s\ ^2S_{1/2}$	$5p\ ^2P_{3/2}$	83.5696	0.9803	9.362*E*+11
$3d\ ^2D_{5/2}$	$6p\ ^2P_{3/2}$	75.9259	0.0060	6.961*E*+09
$2d\ ^2D_{3/2}$	$6p\ ^2P_{1/2}$	75.9001	0.0033	3.871*E*+09
$3d\ ^2D_{3/2}$	$6p\ ^2P_{3/2}$	75.8830	0.0007	7.747*E*+08
$3d\ ^2D_{5/2}$	$6f\ ^2F_{5/2}$	75.7751	0.0154	1.795*E*+10
$3d\ ^2D_{5/2}$	$6f\ ^2F_{7/2}$	75.7724	0.3090	3.589*E*+11
$3d\ ^2D_{3/2}$	$6f\ ^2F_{5/2}$	75.7323	0.2164	2.517*E*+11
$3p\ ^2P_{3/2}$	$6s\ ^2S_{1/2}$	75.1995	0.0163	1.922*E*+10
$3p\ ^2P_{1/2}$	$6s\ ^2S_{1/2}$	75.0650	0.0082	9.659*E*+09
$3p\ ^2P_{3/2}$	$6d\ ^2D_{3/2}$	74.6989	0.0223	2.667*E*+10
$3p\ ^2P_{3/2}$	$6d\ ^2D_{5/2}$	74.6937	0.2008	2.401*E*+11
$3p\ ^2P_{1/2}$	$6d\ ^2D_{3/2}$	74.5662	0.1118	1.341*E*+11
$3s\ ^2S_{1/2}$	$6p\ ^2P_{1/2}$	71.8651	4.7971	6.195*E*+12
$3s\ ^2S_{1/2}$	$6p\ ^2P_{3/2}$	71.8498	9.5962	1.240*E*+13
$3d\ ^2D_{5/2}$	$7p\ ^2P_{3/2}$	69.7071	0.0030	4.124*E*+09
$3d\ ^2D_{3/2}$	$7p\ ^2P_{1/2}$	69.6800	0.0017	2.294*E*+09
$3d\ ^2D_{3/2}$	$7p\ ^2P_{3/2}$	69.6709	0.0003	4.589*E*+08
$3d\ ^2D_{5/2}$	$7f\ ^2F_{5/2}$	69.6272	0.0073	1.009*E*+10
$3d\ ^2D_{5/2}$	$7f\ ^2F_{7/2}$	69.6258	0.1467	2.019*E*+11
$3d\ ^2D_{3/2}$	$7f\ ^2F_{5/2}$	69.5911	0.1028	1.415*E*+11
$3p\ ^2P_{3/2}$	$7s\ ^2S_{1/2}$	68.9768	0.0084	1.177*E*+10
$3p\ ^2P_{1/2}$	$7s\ ^2S_{1/2}$	68.8636	0.0042	5.916*E*+09
$3p\ ^2P_{3/2}$	$7d\ ^2D_{3/2}$	68.7119	0.0116	1.640*E*+10
$3p\ ^2P_{3/2}$	$7d\ ^2D_{5/2}$	68.7091	0.1045	1.477*E*+11
$3p\ ^2P_{1/2}$	$7d\ ^2D_{3/2}$	68.5996	0.0582	8.243*E*+10
$3s\ ^2S_{1,2}$	$7p\ ^2P_{1/2}$	66.2644	0.5981	9.085*E*+11
$3s\ ^2S_{1/2}$	$7p\ ^2P_{3/2}$	66.2562	1.1964	1.818*E*+12
$2p\ ^2P_{3/2}$	$3s\ ^2S_{1/2}$	45.5964	0.0824	2.644*E*+11
$2p\ ^2P_{1/2}$	$3s\ ^2S_{1/2}$	45.4292	0.0414	1.336*E*+11
$2p\ ^2P_{3/2}$	$3d\ ^2D_{3/2}$	44.1087	0.2704	9.269*E*+11
$2p\ ^2P_{3/2}$	$3d\ ^2D_{5/2}$	44.0942	2.4342	8.350*E*+12
$2p\ ^2P_{1/2}$	$3d\ ^2D_{3/2}$	43.9521	1.3567	4.684*E*+12
$2s\ ^2S_{1/2}$	$3p\ ^2P_{1/2}$	40.8703	0.0169	6.750*E*+10
$2s\ ^2S_{1/2}$	$3p\ ^2P_{3/2}$	40.8305	0.0338	1.354*E*+11
$2p\ ^2P_{3/2}$	$4s\ ^2S_{1/2}$	33.2577	0.0172	1.040*E*+11
$2p\ ^2P_{1/2}$	$4s\ ^2S_{1/2}$	33.1686	0.0086	5.241*E*+10
$2p\ ^2P_{3/2}$	$4d\ ^2D_{3/2}$	32.9226	0.0493	3.033*E*+11
$2p\ ^2P_{3/2}$	$4d\ ^2D_{5/2}$	32.9192	0.4437	2.731*E*+12
$2p\ ^2P_{1/2}$	$4d\ ^2D_{3/2}$	32.8253	0.2471	1.529*E*+12
$2s\ ^2S_{1/2}$	$4p\ ^2P_{1/2}$	30.9674	0.1288	8.960*E*+11
$2s\ ^2S_{1/2}$	$4p\ ^2P_{3/2}$	30.9578	0.2577	1.794*E*+12
$2p\ ^2P_{3/2}$	$5s\ ^2S_{1/2}$	29.6011	0.0067	5.119*E*+10
$2p\ ^2P_{1/2}$	$5s\ ^2S_{1/2}$	29.5305	0.0034	2.578*E*+10
$2p\ ^2P_{3/2}$	$5d\ ^2D_{3/2}$	29.4659	0.0182	1.399*E*+11
$2p\ ^2P_{3/2}$	$5d\ ^3D_{5/2}$	29.4645	0.1639	1.260*E*+12

(Continued)

transition $n'l'^2L'_j \leftarrow nl^2L_j$		wavelangth λ(Å)	oscillator strength gf(au)	transition probabilites gA(sec^{-1})
$2p\ ^2P_{1/2}$	$5d\ ^2D_{3/2}$	29.3959	0.0913	7.047E+11
$2p\ ^2P_{3/2}$	$6s\ ^2S_{1/2}$	27.9459	0.0034	2.894E+10
$2p\ ^2P_{1/2}$	$6s\ ^2S_{1/2}$	27.8830	0.0017	1.457E+10
$2p\ ^2P_{3/2}$	$6d\ ^2D_{3/2}$	27.8765	0.0089	7.674E+10
$2p\ ^2P_{3/2}$	$6d\ ^2D_{6/2}$	27.8758	0.0805	6.907E+11
$2s\ ^2S_{1/2}$	$5p\ ^2P_{1/2}$	27.8563	0.0144	1.236E+11
$2s\ ^2S_{1/2}$	$5p\ ^2P_{3/2}$	27.8523	0.0288	2.474E+11
$2p\ ^2P_{1/2}$	$6d\ ^2D_{3/2}$	27.8139	0.0448	3.863E+11
$2p\ ^2P_{3/2}$	$7s\ ^2S_{1/2}$	27.0394	0.0020	1.798E+10
$2p\ ^2P_{3/2}$	$7d\ ^2D_{3/2}$	26.9986	0.0051	4.683E+10
$2p\ ^2P_{3/2}$	$7d\ ^2D_{6/2}$	26.9982	0.0461	4.215E+11
$2p\ ^2P_{1/2}$	$7s\ ^2S_{1/2}$	26.9805	0.0010	9.047E+09
$2p\ ^2P_{1/2}$	$7d\ ^2D_{3/2}$	26.9399	0.0256	2.357E+11
$2s\ ^2S_{1/2}$	$6p\ ^2P_{1/2}$	26.4183	0.2556	2.442E+12
$2s\ ^2S_{1/2}$	$6p\ ^2P_{3/2}$	26.4163	0.5112	4.886E+12
$2s\ ^2S_{1/2}$	$7p\ ^2P_{1/2}$	25.6222	0.0000	0.000E+00
$2s\ ^2S_{1/2}$	$7p\ ^2P_{3/2}$	25.6210	0.0000	0.000E+00

对于已实现软 X 射线激光的跃迁 $5f$–$3d$, $5d$–$3p$, $6f$–$3d$ 及 $6d$–$3p$, 把纯理论计算波长与实验值作一比较，如表 3 所列，其相对误差均小于 0.1%。24 条谱线(类锂硅离子)数据作了比较，如表 4 所列。两者基本相符，相对误差不超过 1%。这说明本文的计算结果是可信的。

Table 3　Comparison of theoretical and experimental transition wavelengths of Li-like Si XII soft X-ray lasers

transition	theoretical wavelength (Å)	experimental wavelengths(Å)
5f - 3d	88.754	88.84
5d - 3p	87.256	87.28
6f - 3d	75.760	75.83
6d - 3p	74.653	74.64

四、结　论

本文给出了理论计算得到的类锂硅离子 $1s^2nl$($2 \leqslant n \leqslant 7$)各能级平均能量及在波长小于 400Å 范围内 $1s^2nl^2L_j$—$1s^2n'l'^2L'_j$ 跃迁各谱线光谱性质：波长、振子强度和跃迁几率。其中波长在理论上精度误差不超过 1%。这些数据对等离子体光谱识别及软 X 射线激光研究都是十分有用的。

对已实现 X 射线激光的跃迁 $5f$–$3d$, $5d$–$3p$, $6f$–$3d$ 及 $6d$–$3p$, 理论计算得到的波长与实验值完全相符。本文给出了 $7f$–$3p$ 和 $7d$–$3p$ 跃迁的理论数据，软 X 射线激光实验可以作

Table 4 Comparison of calculated and existing in R. L. Kelly[12] transition wavelengths in Si XII

transition $1S^2n\ l\ ^{12}Li$--$1S^2nl'\ ^2Li$	calculated λ(Å)	R.L.Kelly λ'(Å)
2S $^2S_{1/2}$ 7p $^2P_{3/2}$	25.6210	25.655
2S $^2S_{1/2}$ 6p $^2P_{3/2}$	26.4163	26.460
2p $^2P_{1/2}$ 7d $^2D_{3/2}$	26.9399	26.98
2p $^2P_{3/2}$ 7d $^2D_{5/2}$	26.9982	27.035
2p $^2P_{1/2}$ 6d $^2D_{3/2}$	27.8139	27.850
2p $^2P_{3/2}$ 6d $^2D_{5/2}$	27.8758	27.909
2p $^2P_{1/2}$ 5d $^2D_{3/2}$	29.3959	29.439
2p $^2P_{3/2}$ 5d $^2D_{5/2}$	29.4645	29.509
2p $^2P_{1/2}$ 5s $^2S_{1/2}$	29.5305	29.547
2p $^2P_{3/2}$ 5s $^2S_{1/2}$	29.6011	29.645
2s $^2S_{1/2}$ 4p $^2P_{3/2}$	30.9578	31.015
2p $^2P_{1/2}$ 4d $^2D_{3/2}$	32.8353	32.888
2p $^2P_{1/2}$ 4d $^2D_{5/2}$	32.9192	32.972
2s $^2S_{1/2}$ 3p $^2P_{3/2}$	40.8305	40.911
2s $^2S_{1/2}$ 3p $^2P_{1/2}$	40.8703	40.951
2p $^2P_{1/2}$ 3d $^2D_{3/2}$	43.9521	44.021
2p $^2P_{3/2}$ 3d $^2D_{5/2}$	44.0942	44.165
2p $^2P_{1/2}$ 3s $^2S_{1/2}$	45.4292	45.519
2p $^2P_{3/2}$ 3s $^2S_{1/2}$	45.5964	45.629
3d $^2D_{5/2}$ 5f $^2F_{7/2}$	88.7688	88.84
3p $^2P_{1/2}$ 4d $^2D_{3/2}$	126.3804	126.43
3p $^2P_{3/2}$ 4d $^2D_{5/2}$	126.7116	126.77
3d $^2D_{3/2}$ 4f $^2F_{5/2}$	129.6253	129.89
3d $^2D_{5/2}$ 4f $^2F_{7/2}$	129.7241	130.02

这方面的尝试，向波长更短的激光推进，以更接近“水窗”。

在本文研究过程中，对张正泉、范品忠和陈时胜等教授曾予讨论和有益的建议，陆培祥、李跃林及马锦秀等同志的共同讨论也使我们得益匪浅，在此特致谢意！另外，也感谢郑丹青同志在调试和使用 Cowan 程序中给予帮助。

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Li-like Si ions energy level structure and Ab initio Si XII spectral calculation

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Abstract

Relative energies of every Li-like Si ions energy level ($n=2\sim7$) and ab initio Si XII wavelengths below 400Å involving transitions between $1s^2nl^2L$, levels up to $n=7$ are calculated. Corresponding transition probabilities and line strengths are given. The accuracy of wavelength calculation is better than 1% comparing with existing data. The calculated wavelengths of Si XII $5d$–$3p$, $5f$–$3d$, $6d$–$3p$ and $6f$–$3d$ transitions are in good agreement (within 0.1%) with the observed transition wavelengths at which soft X-ray lasers have been experimentally demonstrated. The Si XII $7d$–$3p$ and $7f$–$3d$ transitions are of potential interest for X-ray lasers with shorter wavelengths towards the Water Window.

Key words: Li-like Si ions= Ab initio Si XII spectra.