

FIRST PRINCIPLE CALCULATIONS OF DEFECT STRUCTURES
IN ZINC OXIDE

By

CHRISTIAN LOER T. LLEMIT

A thesis submitted in partial fulfillment of
the requirements for the degree of

BACHELOR OF SCIENCE

UNIVERSITY OF THE PHILIPPINES - DILIMAN
National Institute of Physics

MAY 2020

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To the Faculty of University of the Philippines Diliman National Institute of Physics:

The members of the Committee appointed to examine the thesis of CHRISTIAN LOER
T. LLEMIT find it satisfactory and recommend that it be accepted.

Roland V. Sarmago, Ph.D., Chair

Donald Trump, Ph.D.

Rodrigo Duterte, Ph.D.

ACKNOWLEDGMENT

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FIRST PRINCIPLE CALCULATIONS OF DEFECT STRUCTURES
IN ZINC OXIDE

Abstract

by Christian Loer T. Llemit, BS
University of the Philippines - Diliman
May 2020

: Roland V. Sarmago

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Dedication

This dissertation/thesis is dedicated to my mother and father who
provided both emotional and financial support

Chapter One

INTRODUCTION

1.1 Semiconductors

1.2 Applications of Semiconductors

1.3 Defects in Semiconductors

1.4 ZnO

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1.4.1 Subsection of section - double quotes

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1.4.2 Another subsection of section - citations

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Example of multiple citations [3, 4]. Nullam mollis et leo at pharetra. Nulla efficitur molestie euismod. Sed dapibus metus sed tempus varius. Aenean finibus eros ut urna luctus feugiat. Duis turpis risus, viverra vitae porta et, ullamcorper ac est. Proin in eros nec ipsum interdum tempus. Nam fringilla lectus velit, non posuere ex vehicula ut. Mauris tincidunt, dolor sit amet commodo tempor, erat mi egestas dui, at elementum tellus est rhoncus libero. Ut et rutrum lectus, id viverra tortor. Vivamus nec lacus eros. Donec dictum porta nisi et vestibulum. Mauris luctus ligula ut libero aliquet luctus. Quisque malesuada egestas finibus.

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lorem auctor. Pellentesque finibus elit justo, a vulputate diam fermentum lacinia.

Chapter Two

THEORETICAL FRAMEWORK

2.1 Many-body Quantum Mechanics

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2.1.1 Simplifying Assumptions

2.1.2 Time Independent Schrödinger Equation

2.1.3 Use of Atomic Units

2.1.4 Hamiltonian Operator

2.1.5 Indistinguishability of electrons

2.2 Early First Principle Calculations

2.2.1 n-electron problem

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2.3 Density Functional Theory

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2.3.2 Hohenberg-Kohn (HK) Formalism

2.3.2.1 First HK Theorem

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2.3.3 Kohn Sham (KS) Formalism

2.3.3.1 KS Equation

2.3.3.2 Energy Terms

2.4 Exchange-correlation Functional

2.4.1 Local Density Approximation (LDA)

Chapter Three

DFT Calculation of Solids

3.1 Pseudopotential Approach

This is sample text

3.1.1 Freezing the core electrons

3.1.2 Pseudizing the valence electrons

3.1.3 Common Pseudopotentials

3.2 Choosing the appropriate Calculation Size

3.2.1 Use of Supercell

3.2.1.1 Periodic Boundary Conditions (PBC)

3.2.2 Use of Reciprocal Space

3.2.2.1 Reciprocal Lattice

3.2.2.2 First Brillouin Zone

3.2.2.3 Irreducible Brillouin Zone

3.2.3 k-point sampling

3.2.3.1 Monkhorst-Pack method

3.2.3.2 Gamma Point Sampling

Example of double quotes “word”. Lore

3.3 Bloch Representations

3.3.1 Electrons in solid

3.3.2 Bloch Theorem in periodic systems

3.3.3 Fourier Expansion of Bloch representations

3.3.3.1 Fourier Expansions

3.3.3.2 Fast Fourier Transformation (FFT)

3.3.3.3 Kohn-Sham Matrix Representations

3.4 Plane Wave (PW) Expansion

3.4.1 Basis Set

3.4.1.1 Local Basis Set

3.4.1.2 Plane Wave Basis Set

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3.5.1 Band Structure of free electrons

3.5.2 Band Structure of electrons in solids

3.5.3 Electronic Density of States

3.6 Practical Aspects

Chapter Four

MATHEMATICS NOTATION

4.1 Some Math Stuff

LaTeX has a special way to embed mathematical symbols and notations. Here are some of them. Also observe how a bullet list is made.

- greater than \geq
- less than \leq
- percent sign %
- multiply $N \times N$
- inline equation $M = N(N - 1)/2$

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4.2 Math equation

Example of a mathematical formula:

$$ADD = \sum_{i=1}^M | < D(n+1, i) > - < D(n, i) > | \quad (4.1)$$

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4.3 Chapter section

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Chapter Five

FIGURES AND TABLES

5.1 Examples of a figure

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Example of a figure. Example of reference to a figure in the text (Fig. 5.1). Phasellus dolor neque, vehicula vestibulum semper at, facilisis eget libero. Mauris interdum magna molestie, auctor felis a, condimentum odio. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Suspendisse maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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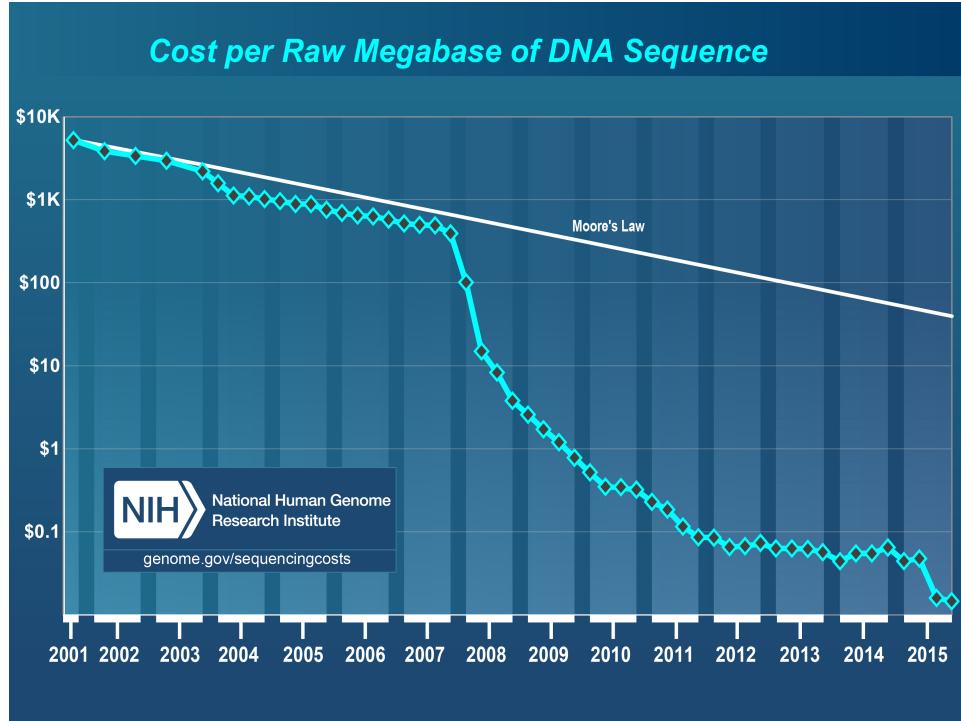


Figure 5.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]

5.2 Example of a table

Example of a table and here is the reference to Table 5.1. Tables in, my opinion, are the hardest thing to make.

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ORGANISM	ACCESSION NO.	GENOME SIZE (bp)	No. CDS
<i>Mesorhizobium loti</i>	NC_002678	7036071	6743
<i>Sinorhizobium meliloti</i>	NC_003047	3654135	3359
<i>Bradyrhizobium japonicum</i>	NC_004463	9105828	8317
<i>Rhodopseudomonas palustris</i>	NC_005296	5459213	4813
<i>Bartonella quintana</i>	NC_005955	1581384	1142
<i>Bartonella henselae</i>	NC_005956	1931047	1488
<i>Rickettsia typhi</i>	NC_006142	1111496	837
<i>Beijerinckia indica</i>	NC_010581	4170153	3569

Table 5.1 Whole-genome sequences used in this study

sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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5.3 Chapter section

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maximus lacinia dignissim. Maecenas pharetra accumsan metus, sagittis dictum purus sollicitudin eget. Curabitur ut porttitor arcu, ut porttitor ipsum. Vestibulum porttitor finibus sapien, ac pharetra odio bibendum nec. Nullam tincidunt dignissim risus imperdiet dictum.

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APPENDIX

Appendix A

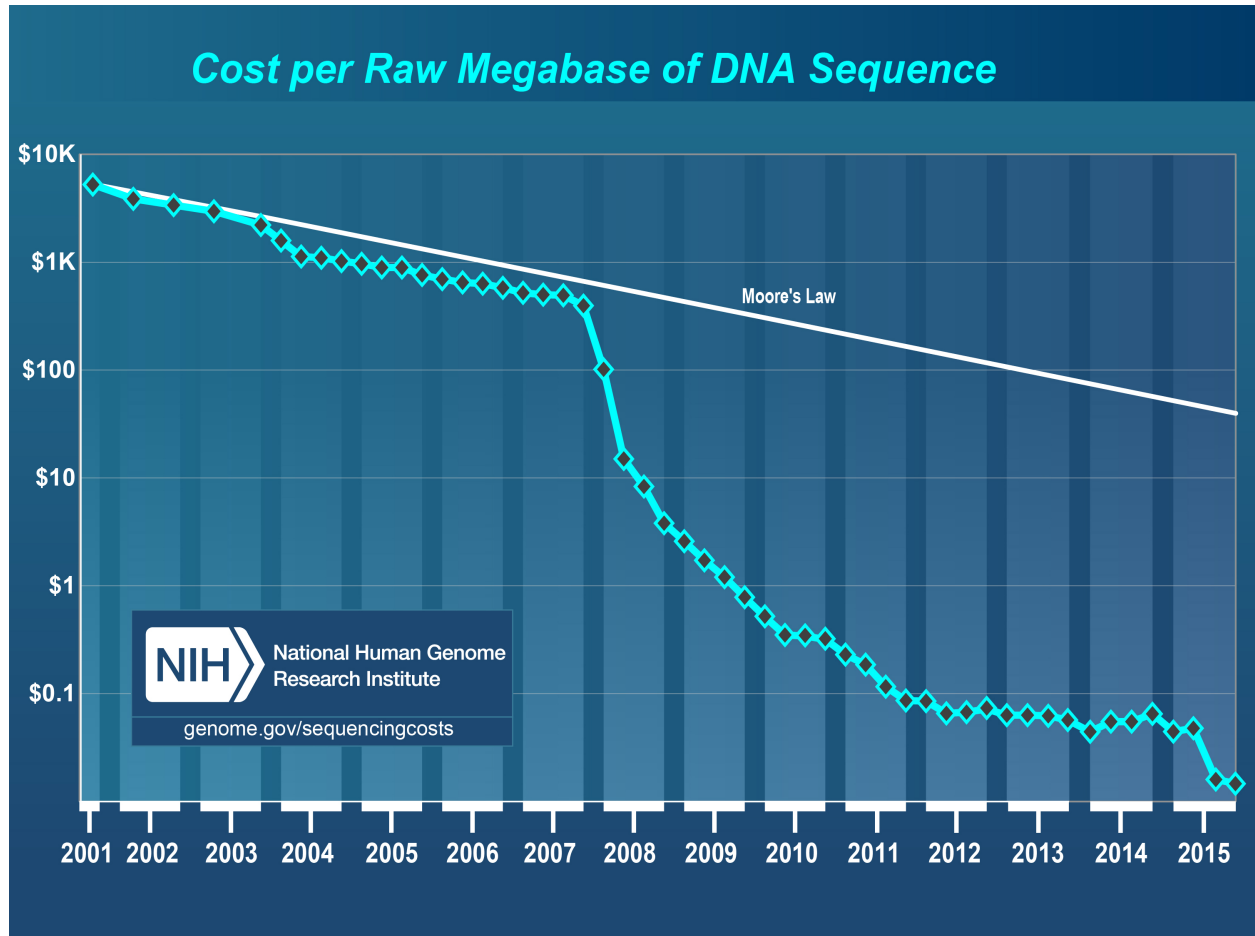


Figure A.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]

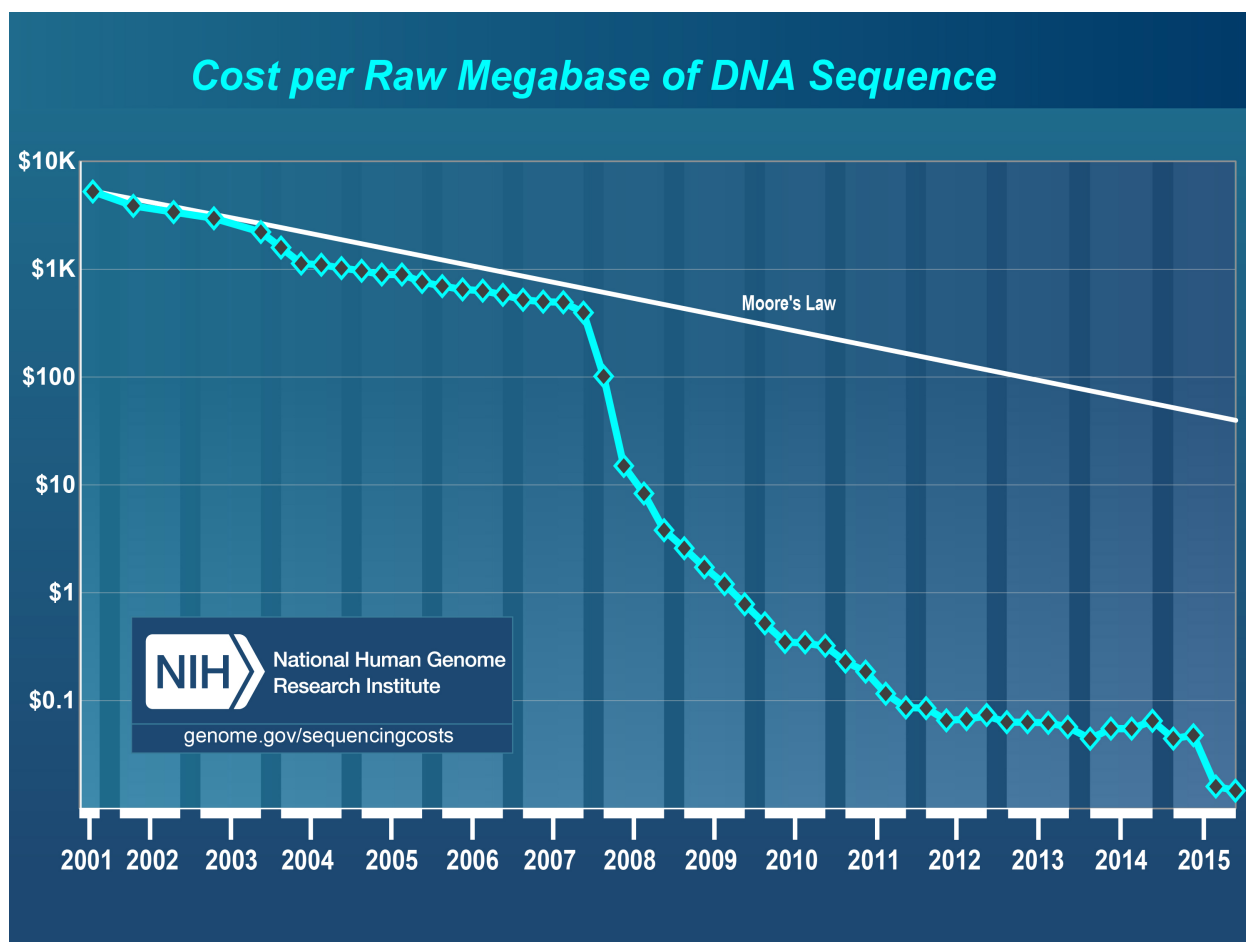


Figure A.2 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]

Appendix B

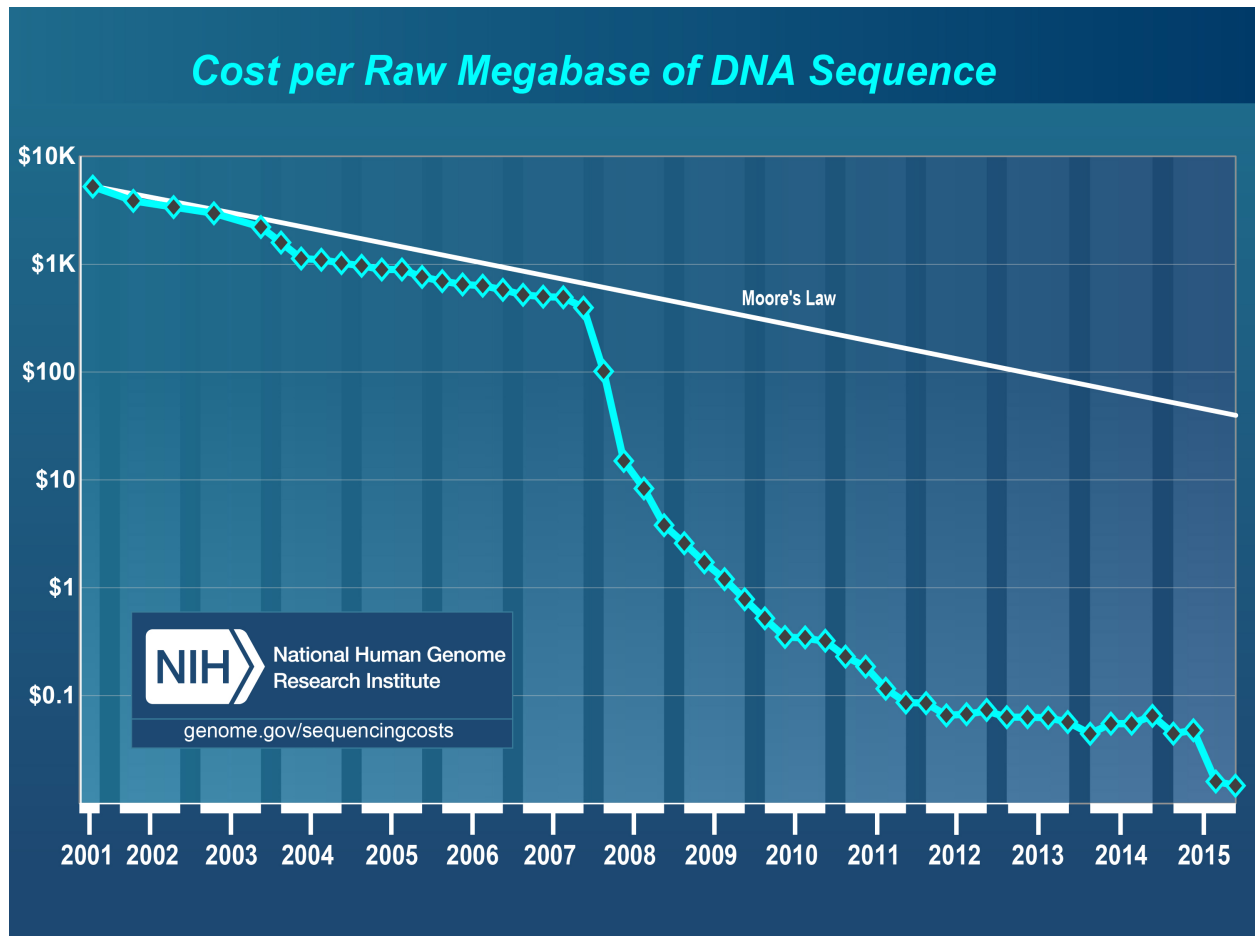


Figure B.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]

Appendix C

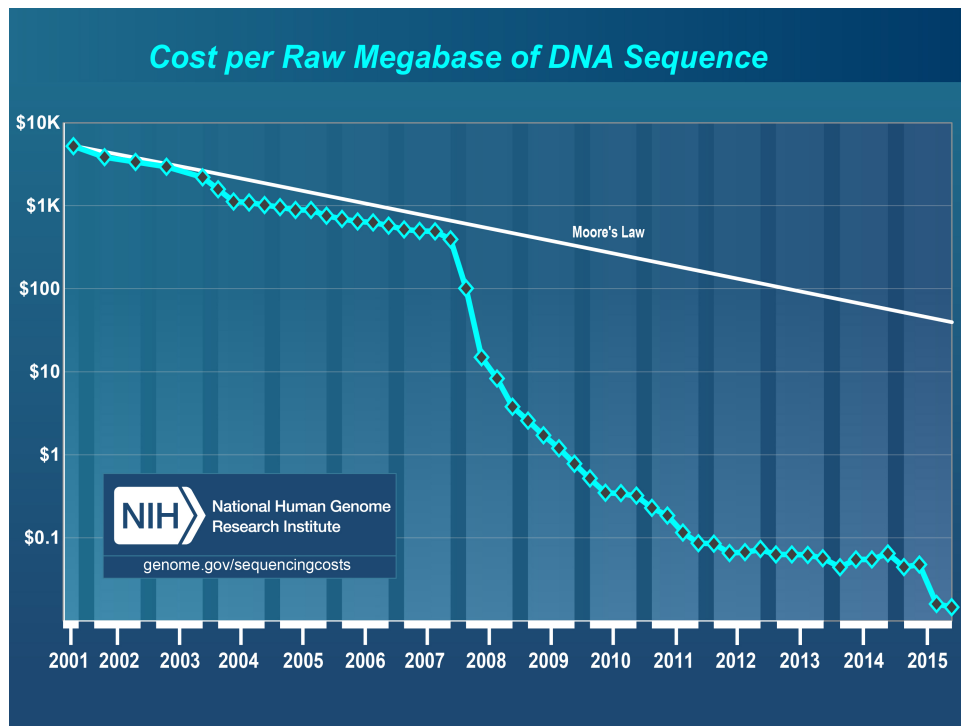


Figure C.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]

Appendix D

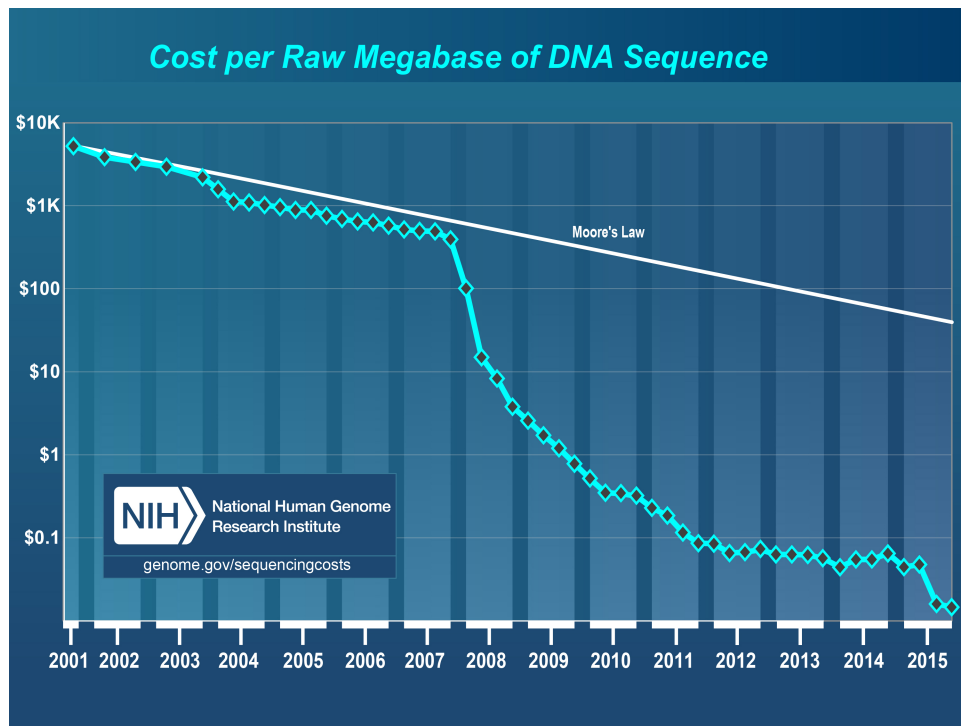


Figure D.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]

Appendix E

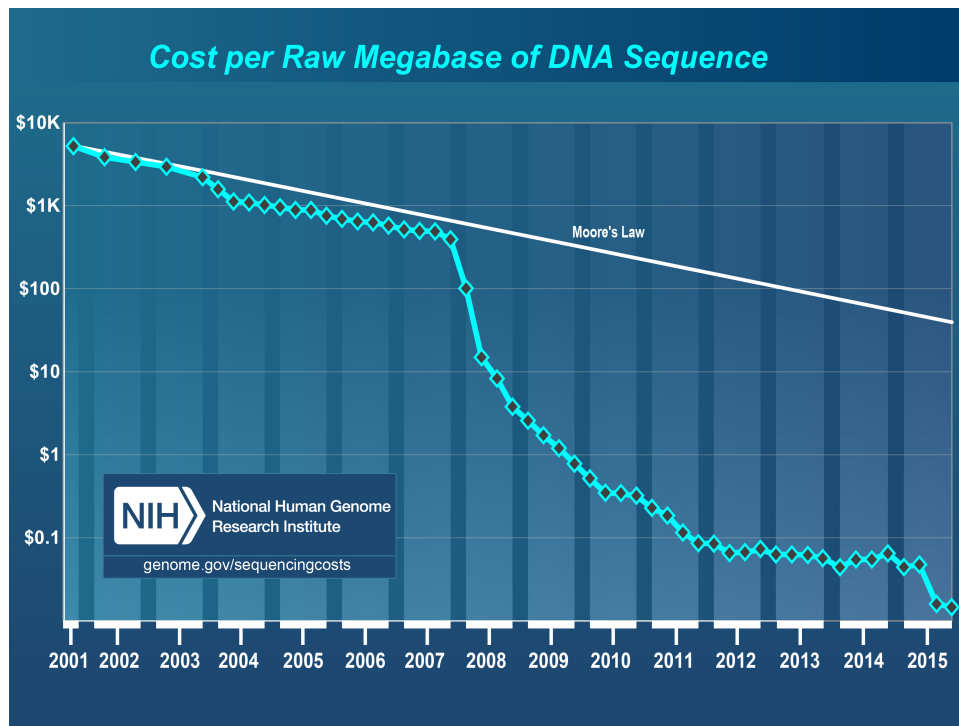


Figure E.1 Cost per raw megabase of DNA sequence from 2001 to 2015. Straight line - Moore's Law, blue curve - cost in US dollars, Y-axis scale is logarithmic. Graph reproduced from [5]